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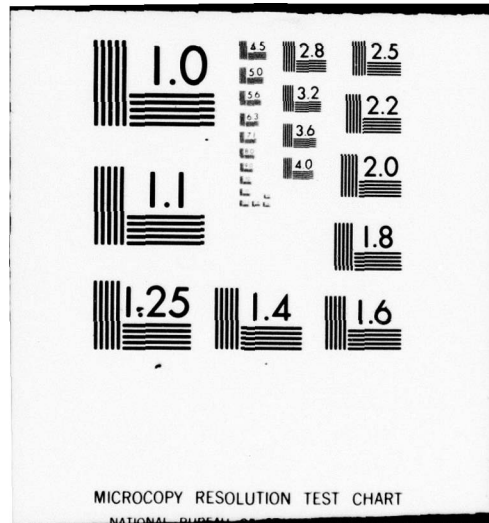
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AN INTRODUCTION TO STATISTICAL  
DESIGN OF EXPERIMENTS  
IN METALLURGICAL RESEARCH

By S. J. Hussey, P. L. Plascik, and C. H. Schack

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UNITED STATES DEPARTMENT OF THE INTERIOR  
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By S. J. Hussey, P. L. Placek, and C. H. Schack

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# AN INTRODUCTION TO STATISTICAL DESIGN OF EXPERIMENTS IN METALLURGICAL RESEARCH<sup>1</sup>

by

S. J. Hussey,<sup>2</sup> P. L. Placek,<sup>3</sup> and C. H. Schack<sup>4</sup>

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## SUMMARY

↙ This Bureau of Mines report presents a discussion of the statistical approach to the design of experiments and indicates, by concrete examples, how and when statistical design is essential for obtaining meaningful data with a minimum number of experiments.

↗ Every research worker plans his work and designs his experiments in a manner which, based on his experience, seems most rational to him and which he believes will produce the information essential for resolving the problems. If the results obtained are open to multiple interpretations and are not of definitive reliability, the failure of the experiment design to produce the desired information may be due to several causes. These include faulty judgment in selecting the factors to be tested, ignoring the importance of interaction between factors, failure to adequately control test variables, and assuming that meaningful trends in the results can be identified without comparison to a predetermined experimental error. An experienced researcher probably will deduce from the nature of the data obtained that the design is faulty and may by trial and error ultimately arrive at the correct solution to the problem. Statistical methods of planning research minimize the chance of faulty experiment design, embody concrete procedures for testing the validity and reliability of the test data and for indicating mandatory changes in the design, and enable the researcher to obtain meaningful information with the least number of tests.

The classical or "Edisonian" method of designing a research program is the essence of simplicity. Each factor deemed to have a significant influence on the results is separately investigated. The effect of each factor is estimated by a series of tests which vary one factor over a selected range of

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<sup>1</sup>Work on manuscript completed August 1962.

<sup>2</sup>Supervising metallurgist, Salt Lake City Metallurgy Research Center, Bureau of Mines, Salt Lake City, Utah.

<sup>3</sup>Extractive metallurgist, Salt Lake City Metallurgy Research Center, Bureau of Mines, Salt Lake City, Utah.

<sup>4</sup>Supervising research metallurgist, Salt Lake City Metallurgy Research Center, Bureau of Mines, Salt Lake City, Utah.

values while holding all other factors constant. Such a design of the experimental work will be adequate for the investigation of problems involving simple relationships or for research directed to achieve goals readily identified by data that may lack specified precision and reliability. When, as is common, the research involves complex interrelationships between many diverse factors, definitive trends and conclusions can be made only from data that can be analyzed and tested as to validity and significance. An experimental design based on the classical method, however, will not detect or yield estimates of significant interaction effects between the important factors, nor can the data be objectively analyzed to provide information as to reliability.

The purpose of statistical design is to plan experiments so that the results will yield meaningful information about fundamental or empirical relationships. Statistical methods embody well codified designs for various types of experimental conditions and also provide ways to determine the merits of such designs for providing information in research. Overdesign and underdesign are inevitable unless suitable criteria are used to judge the correct number and type of observations to make.

The designs discussed in this report are for (1) estimating the effect of one or more independent variables upon a dependent variable and (2) defining an equation by which the dependent variable can be estimated from values of the independent variables. In the statistical approach to research, the postulation that the dependent and the independent variables determine a hypothetical and mathematical space provides the theoretical setting for the development of mathematical expressions for empirical and fundamental relationships. The use of statistical principles within such settings facilitates the development of the desired equations that represent the relationships being investigated.

One of the more important statistical designs is the factorial design by means of which several factors and their interactions are studied. Two-level factorial designs are particularly applicable in preliminary research and in the determination of optimum operating conditions. Factorial designs in which more than two levels are selected for some or all of the factors are used when a more complete investigation of the relationships between factors and response is desired. When main effects are not linear over the region of interest and interaction effects are relatively large, more than two levels for the factors are necessary for a complete study of the response.

A fractional factorial design may be used when some of the interactions are not important. In such a design the estimates of the various effects are combined so that only the important effects are studied in an experiment. When the estimates of effects are thus combined, they are said to be confounded. The tests which are sufficient for estimating the important effects are selected from the corresponding full factorial design. Fractional factorial designs and the principle of confounding also are useful in metallurgical research when it is necessary to introduce minor factors into an experiment by making tests in two or more sets which are called blocks. Tests are assigned to the different blocks in such a way that the effects of these minor factors will be confounded with unimportant interaction effects. When all the



interactions between factors are important, several experiments should be made in which the effect of a difference between two blocks is confounded with a different interaction effect in each experiment. Thus, an estimate of every interaction effect is obtained from at least one experiment. This procedure is called partial confounding.

The selection of a sufficient number of factor levels for investigation in an experiment is important. When insufficient levels are selected, important polynomial components that are not taken into consideration are confounded with those polynomial components for which the design was prepared. The estimates of the latter components then are biased. In such a situation an economy sometimes can be effected in the amount of experimental work by making a few additional tests properly related to the tests of the basic factorial or fractional factorial design without making a full factorial design of higher order. Such designs are termed composite designs and provide the advantage of proceeding with experimental work by natural stages. The composite design is especially helpful in the determination of optimum conditions by taking the shortest route as determined by a succession of two-level factorial experiments.

Nested designs generally are used when successive sampling is necessary to determine the variation in some characteristic that contributes to the experimental error. By means of nested designs the total experimental error may be divided into components corresponding to the errors contributed by several sources. Multiple replication at any level in a design is made to increase the precision of estimating effects and should not be used solely to obtain a better estimate of experimental error.

When an experiment is designed by statistical methods, the experimental errors that are associated with each observation are assumed to be random variables that are uncorrelated between replicates and between factor levels. Correlation due to factors that cannot be controlled may be minimized by randomization in the execution of the experiment. Correlation between errors may cause trends in the results that contribute to the estimates of important effects.

Precise formulation of experiment objectives and adequate design of experiments followed by capable analysis of data are characteristics of well executed research. One of the most valuable benefits resulting from the use of statistical methods is an enforced discipline of thought leading to a precise formulation of research problems and experimental objectives. This is the foundation upon which the statistical design of experiments is based. A later report is planned to consider the methods used in analyzing data from statistically designed experiments.

## INTRODUCTION

The studies herein reported were undertaken as a part of a broader Bureau of Mines program on the application of statistical methods to planning and evaluating research in extractive metallurgy. Research has become increasingly dependent upon the services of skilled and semiskilled technicians guided by a



limited professional staff. Therefore, it has become imperative to utilize every possible means of increasing the efficiency and effectiveness of planning, directing, conducting, and evaluating the research program. This report is intended primarily for the benefit of research workers with professional training who must first design and direct experiment work and then evaluate the resulting data in terms of comprehensive and meaningful results.

Statistical theory is a branch of applied mathematics that has its roots in the area of pure mathematics known as the theory of probability. In applying statistical methods, the research worker uses mathematical tools that have been devised to facilitate the analysis of data and the design and analysis of various types of experiments. Most books written on statistical methods and their practical application are couched in formidable mathematical terminology or are so abstruse, due to the manner of presenting the illustrative material, that a logical association of the more important and useful principles can be obtained only after extensive study. An attempt has been made in this report to avoid discouraging the researcher who has only an ordinary background in college algebra and an elementary background in calculus.

The salient useful features of statistical methods are the controls which can be exercised over both experiments and deductions with a specified degree of probability. A lack of sufficient control can be determined and the necessary corrective or precautionary measures indicated by statistical methods. These useful features of statistical methods do not obviate the necessity for the research worker to exercise proper judgment in selection of the statistical method best adapted to the particular problem and in the interpretation of the results obtained by statistical analysis. The decisions and conclusions based upon statistical analysis must be properly integrated with the technical knowledge peculiar to each investigation.

In presenting a coherent discussion of so complex a subject as the application of statistical methods to the design of metallurgical research, considerable simplification has been necessary. Only those elements of probability theory sufficient to enable the reader to understand the principles involved in statistical design are presented. Words that have a unique meaning in statistical mathematics are defined. Special attention is given to presenting the symbolic language of statistics in a consistent and clear manner readily coordinated with that used in important references cited in this report. Finally, the report attempts to illustrate by means of concrete examples of metallurgical problems when and how different statistical methods can be used to design the simplest and most efficient experiment program that will produce meaningful data readily analyzed to derive conclusions with a specified degree of probability.

#### DESIGN OF EXPERIMENTS

A good experimental design is one of three prerequisites to efficient research that will enable the researcher to obtain the information desired with increased effectiveness and with a minimum expenditure of time. The three prerequisites are (1) a correct formulation of the required information, (2) a correct choice of experimental method, after consideration of required

accuracy and experimental pitfalls, and (3) a correct choice of the number and interrelation of the individual tests which characterize the design of the whole experiment. These prerequisites should be considered in the sequence listed, since the first two steps will affect the usefulness of the design.

Statistical design basically deals with the third prerequisite for obtaining maximum results from a minimum of experimental work. Statistical methods have provided (1) well codified designs for various types of experimental conditions, (2) means for determining the relative merits of such designs, and (3) under certain conditions, estimates concerning the necessary number of observations to be made in an experiment. An overdesigned experiment with too many observations results in useless labor. An underdesigned experiment with too few observations may lead to false conclusions. Overdesign and underdesign are inevitable unless a suitable criterion is used to judge the correct number of observations to make. The economies of correct design and a proper number of observations outweigh the extra time and thought required in planning the experiment.

In statistical terminology, dependent variables are called responses because they are results which respond in some manner to changes in the independent variables. In any one experiment there is usually either one such response, or else the results of the experiment can be evaluated independently with respect to each response. The independent variables which affect the response are called factors. Usually many factors influence the response under investigation, and it is essential that all of them be given due consideration. Each factor either should be investigated for its effect upon the response or else should be controlled so that the influence of those factors that are investigated can be independently studied. Due to practical limitations those factors that are considered to have the more important effects upon the response usually are selected for study. Factors such as time, temperature, and concentration are called quantitative factors because they can be classified according to some scale. Factors such as operators, machines, shifts, type of reagent, and type of ore that cannot be defined by a scale are named qualitative factors.

Classifications of a factor in an experiment are called levels. A particular value of the response obtained in an experiment is called an observation. In statistical terminology the combination of all the factor levels in an experiment that produces a particular observation is called a treatment but is herein referred to as a test. An experiment consists of all the tests that are included in the design in order to obtain the desired information.

For the purposes of estimating the experimental error and of obtaining experimental precision, it is often necessary to repeat each test two or more times. An experiment in which every test is performed once is called a single replicate. If every test is performed  $n$  times, then the experiment is said to involve  $n$  replicates. The process of repeating an experiment or a particular test is called replication.

The terms response, factor, quantitative, qualitative, level, test, observation, experiment, and replicate are a convenient means of reference for the detailed discussion of experimental designs and the analysis of results.



The best design for an experiment requires prior knowledge of the errors involved and the size of the effect it is necessary to detect. Even sketchy information is better than none. When statistical design is the operating method of a research center, a store of such knowledge will rapidly accumulate and provide a fund of knowledge for later design work. When such knowledge is sketchy at the start of a research program, further information usually is acquired during the course of the work if proper design has been made. These interim results can be used to provide a more substantial basis for decisions about subsequent design and number of observations. The advantages of this sequential approach are quite marked when it is used in a systematic manner.

The designs that are discussed are for the purpose of estimating the effect of one or more independent variables upon a dependent variable and in many cases to ultimately determine an estimated equation by means of which the dependent variable can be estimated from values of the independent variables. Such designs are based upon the assumption that observing an apparent effect at specific values of the independent variables, with due regard to experimental error, is sufficient grounds to conclude that the dependent variable will be similarly affected for all values in the range of the independent variables involved. There is another class of problems in which the main interest is in determining the existence of a relationship between two or more variables over a specified range with a specified degree of statistical certainty. The statistical procedure for determining these relationships is known as correlation.

#### Mathematical Representation of Natural Relationships

The purpose of statistical design is to provide plans for experiments such that when the experiments are properly executed the results will yield maximum information about fundamental relationships or about empirical relationships that approximate fundamental relationships in a restricted region of the factors. These relationships often are so complex that a study of the underlying causes of all observed effects would involve a prohibitive amount of work. In such cases statistical methods usually can be employed to develop suitable mathematical expressions that represent the natural relationships by means of approximating empirical expressions. Such expressions provide a convenient means of determining optimum conditions for a desired response, a means of predicting values of the response for specific factor combinations, and a means of determining the relative importance of the factors investigated.

#### The Response Surface

In general, the objective of research is to determine the relationships between a response and associated factors in a restricted region bounded by convenient values of the factors. In the statistical approach to research, the response under consideration and the factors chosen for investigation may be considered as variables which determine a hypothetical and mathematical space. Suppose the problem is to define the relationship between the amount of manganese sulfate remaining in solution and the amount precipitated, as affected by the temperature and pH of the solution. The manganese sulfate remaining in solution, the solution pH, and the solution temperature may be represented by axes at right angles as shown in figure 1.

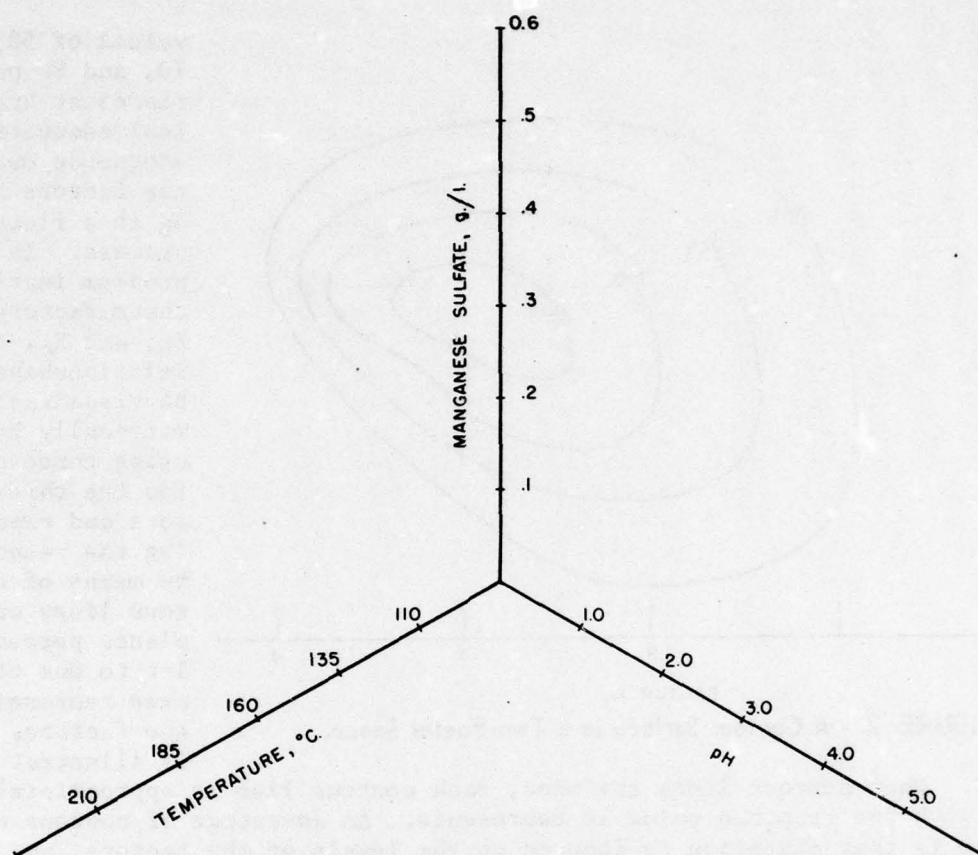


FIGURE 1. - The Geometrical Representation of a Response and Two Factors.

The axes representing manganese sulfate in solution, solution pH, and solution temperature in figure 1 define a hypothetical three-dimensional space. If another factor, such as pressure, were investigated for its effect upon the amount of manganese sulfate in solution, four axes would be necessary for a similar representation, and the problem could not be viewed geometrically. However, in the latter case it is convenient to think of the problem as existing in a hypothetical four-dimensional space. The postulation of such mathematical spaces provides a theoretical setting within which the development of mathematical expressions for empirical and fundamental relationships is made easier. The use of statistical principles within such settings facilitates the development of the desired equations which represent the relationships being investigated.

If values of manganese sulfate in solution were plotted against values of solution pH and solution temperature in figure 1, a curved surface would be obtained. Such a geometrical or hypothetical representation of the relationship between a response and the associated factors is called a response surface. In a problem involving two factors,  $X_a$  and  $X_b$ , the response also may be visualized as contour lines on a plane fixed by the axes representing the two factors. This is illustrated in figure 2. The contour lines with successive



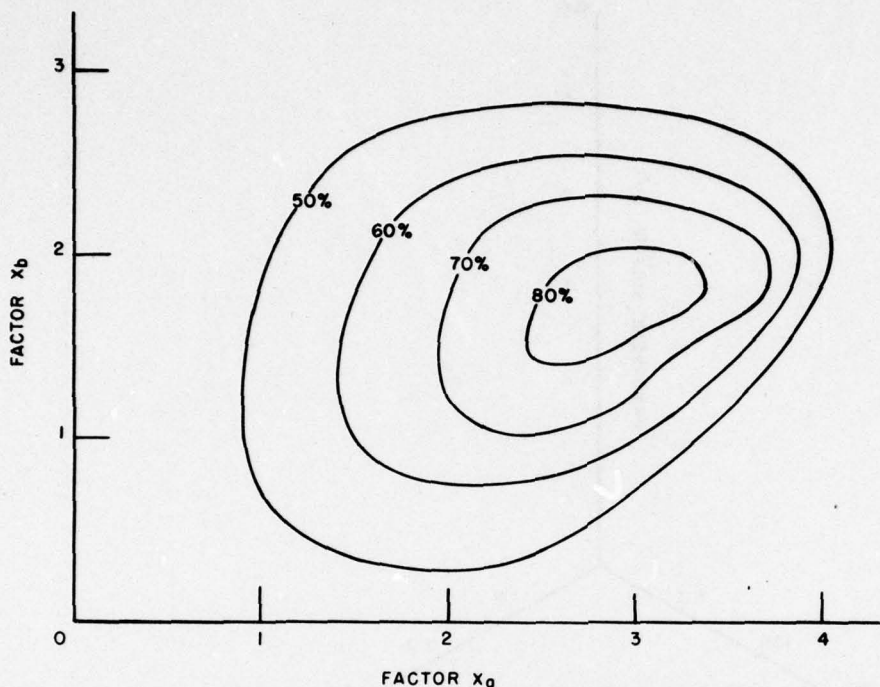


FIGURE 2. - A Contour Surface in a Two-Factor Space.

values of 50, 60, 70, and 80 percent represent hypothetical recoveries of manganese due to the factors  $X_a$  and  $X_b$  in a flotation process. In a problem involving three factors,  $X_a$ ,  $X_b$ , and  $X_c$ , the relationships can be visualized geometrically by using three axes for the three factors and representing the response by means of contour lines on planes perpendicular to one of the axes representing the factors. This is illustrated in

figure 3. When contour lines are used, each contour line is appropriately labeled with the response value it represents. An advantage of contour representation is that attention is focused on the levels of the factors, and the response can be imagined without the distraction of another dimension for the response. In the case of four or more factors, geometrical representation is not possible, and mathematical representation of the hypothetical response surface must be relied upon.

If there are  $p$  factors in an experiment, the mathematical existence of a  $p$ -dimensional space corresponding to the  $p$  factors is implied. This mathematical space is called the factor space. Within the factor space there usually is an approximately defined region corresponding to factor combinations of potential interest. This region is defined by the upper and lower limits of the factors which are of interest to the research worker. This region is called the experimental region and is the region of the factor space within which the research work will be confined, although there may not be any single experiment that will span the whole region.

#### Polynomial Representation

Theoretically any response surface can be represented by some mathematical expression. The proper combination of the factors that produces various levels of the response may be represented by a mathematical expression which is known as the response function. In this paper a factor is represented by the letter  $X$  with appropriate letter subscripts. The general expression for the response obtained in an experiment is the letter  $y$ . This response is

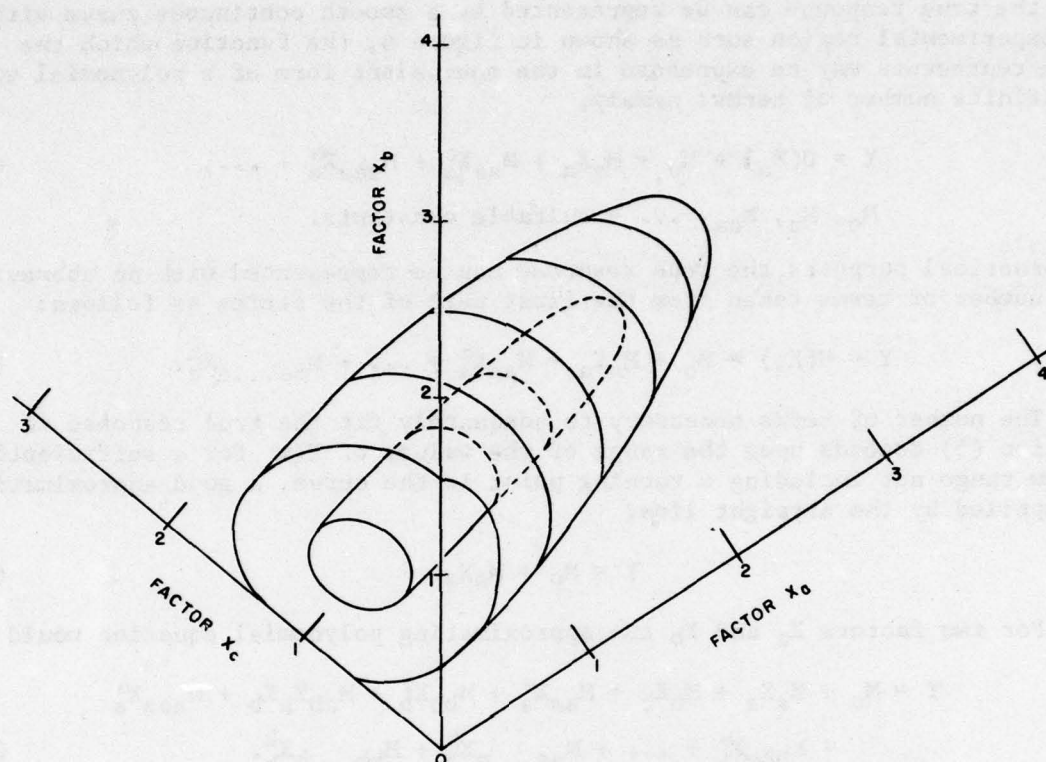


FIGURE 3. - Contour Surfaces in a Three-Factor Space.

statistically considered to be an estimate of the true response, which is represented by the letter  $Y$ . The true response may be considered as the response that could be determined if an infinite number of experiments could be and were made for that purpose. If  $X_a, X_b, \dots, X_k$  are the factors, the relationship between the true response and the factors can be briefly expressed as follows:

$$Y = U(X_a, X_b, \dots, X_k). \quad (1)$$

Equation (1) says that  $Y$  is a function,  $U$ , of the factors  $X_a, X_b, \dots, X_k$ . The function  $U$  is called the true response function. The estimated response function is represented by the letter  $u$  and the relationship between the estimated response,  $y$ , and the estimated response function may be briefly expressed as follows:

$$y = u(X_a, X_b, \dots, X_k). \quad (2)$$

The true response function,  $U$ , may represent for a one-factor problem an exponential relationship such as that shown in figure 4 which is represented by the equation,

$$\begin{aligned} Y = U(X_a) &= Me^{-X_a}, \\ M &= \text{a constant.} \end{aligned} \quad (3)$$

When the true response can be represented by a smooth continuous curve within the experimental region such as shown in figure 4, the function which the curve represents may be expressed in the equivalent form of a polynomial with an infinite number of terms; namely,

$$Y = U(X_a) = M_0 + M_a X_a + M_{aa} X_a^2 + M_{aaa} X_a^3 + \dots, \quad (4)$$

$M_0, M_a, M_{aa}, \dots = \text{suitable constants.}$

For practical purposes the true response can be represented with an abbreviated number of terms taken from the first part of the series as follows:

$$Y = U(X_a) = M_0 + M_a X_a + M_{aa} X_a^2 + \dots + M_{aa \dots a} X_a^k. \quad (5)$$

The number of terms necessary to adequately fit the true response in equation (5) depends upon the range of the values of  $X_a$ . For a sufficiently narrow range not including a turning point in the curve, a good approximation is supplied by the straight line,

$$Y = M_0 + M_a X_a. \quad (6)$$

For two factors  $X_a$  and  $X_b$  the approximating polynomial equation would be

$$Y = M_0 + M_a X_a + M_b X_b + M_{aa} X_a^2 + M_{bb} X_b^2 + M_{ab} X_a X_b + M_{aaa} X_a^3 + M_{bbb} X_b^3 + \dots + M_{aa \dots a} X_a^k + M_{bb \dots b} X_b^k. \quad (7)$$

As in the case of a single factor if the region of the response surface to be represented is small and not near a turning point, then the terms of degree 1 might be sufficient to represent the region. In this case the equation would be

$$Y = M_0 + M_a X_a + M_b X_b. \quad (8)$$

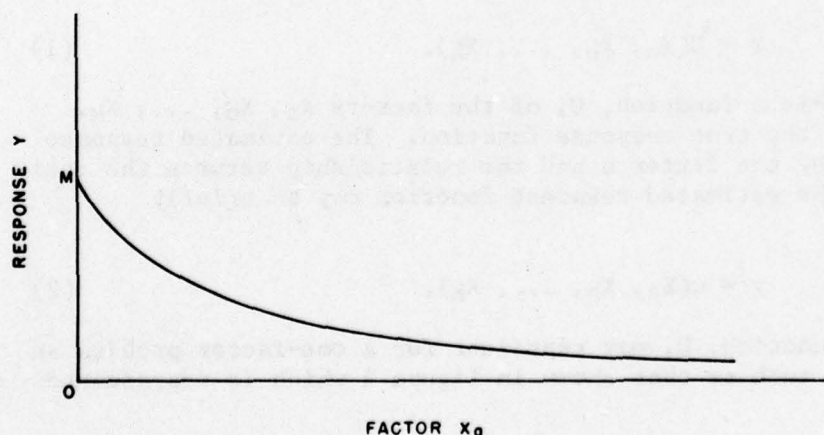


FIGURE 4. - Graph of Response Y for Factor  $X_a$  for the Exponential Relationship,  $Y = Me^{-X_a}$ .

Equation (8) is the equation of a plane in which  $M_a$  represents the slope of the plane in the direction of the factor  $X_a$ , and  $M_b$  represents the slope of the plane in the direction of the factor  $X_b$ . For larger regions or for small regions near a turning point, terms of higher degree would have to be used in order to take into account the curvature of the response surface.



Occasionally it is possible to transform a complex mathematical relationship for a specific problem into a simplified form when prior research has indicated that functions of the dependent or independent variables can be used as the response or factors, respectively, in the design and analysis of an experiment. The use of a function of an independent variable is illustrated by the hypothetical equation,

$$Y = Me^{-T}. \quad (9)$$

Suppose that  $Y$  is the amount of manganese sulfate remaining in solution after thermal precipitation in an autoclave, that  $T$  is temperature ° C., and that equation (9) has been established from prior research. Let it be assumed that further research is being made to investigate the relationship between  $Y$ ,  $T$ , and another factor  $X_b$  which is solution pH. In the investigation it would be reasonable and also helpful to assume the equation,  $Y = U(X_a, X_b)$ , wherein  $X_a = e^{-T}$  rather than  $X_a = T$ . The variable  $e^{-T}$  would be used as a factor in both the design and analysis of the experiments conducted. In the actual conduct of the experiments, the values of  $T$  corresponding to the values of  $e^{-T}$  in the designs would be used. The advantage of this approach is that, in general, it makes possible a closer approximation to the response surface with a smaller number of terms than if temperature itself were used as a factor. The fewer the terms in the response function, the smaller will be the amount of experimental work needed to estimate the values of the coefficients,  $M_i$ , such as those in equation (7).

An example of the advantageous use of a function of the dependent variable for the response,  $Y$ , in a hypothetical flotation experiment follows: Suppose that  $R$  is the recovery of manganese by flotation, that factor  $X_a$  is conditioning time, that factor  $X_b$  is temperature ° C., and that the product variable  $X_a X_b$  is considered to be important in the response function. The true response equation then would be expressed as

$$R = M_0 + M_a X_a + M_b X_b + M_{ab} X_a X_b. \quad (10)$$

However, under certain conditions involving undesirable variations in the experimental error, a different choice of response will eliminate the undesirable variation in the experimental error and also eliminate the necessity for a product term in the response function. In such a case the true response function would be

$$Y = M_0 + M_a X_a + M_b X_b, \quad (11)$$

wherein  $Y = f(R)$  is a function of the recovery which makes a suitable choice of response. The  $M_i$  in equation (11) will not be the same as the  $M_i$  in equation (10). If such information is considered before designing an experiment, the amount of work necessary to conclude the research may be reduced, especially when more than two factors are involved. Examples of functions which might be used in transformations of the response are logarithms, exponentials, sines, cosines, tangents, reciprocals, square roots, and so forth.



### Separation of Response Functions Into Independent Contributions of the Factors

A useful tool of statistical analysis is a procedure for determining the importance of the contribution which the factors in a response function make to the overall variation in the response. This procedure is possible because a response function can be separated into parts which represent the total independent contribution of each factor to the response. The total contribution of a factor to the response is called the effect of the factor. The effect of a factor may be further divided into fractions which can be independently associated with the successive powers of the factor in a response function such as those in equations (7) and (8). These fractions of the effects are herein called polynomial components of the effects. Polynomial components also may be statistically analyzed to determine the importance of the variation in response that may be associated with specific powers of the factors included in the response function. The latter procedure is helpful in determining the nature of the designs that are necessary to conclude additional investigations as quickly as possible with the greatest possible benefit in the form of comprehensive information.

In any experiment the evaluation of the influence of a factor upon the response requires the selection of some standard with which the response at individual levels of the factor can be compared. In a simple one-factor experiment at two levels, a customary comparison is the comparison of the response at the higher level with that at the lower level. For example, if the flotation recovery of zinc using 2 minutes' conditioning time is 85 percent and the recovery using 3 minutes' conditioning time is 89 percent, the metallurgist states that the effect of increasing the conditioning time 1 minute is to increase the zinc recovery by 4 percent. The response at the lower level serves as a standard of comparison for the response at the higher level. If an additional test were made for zinc recovery using 4 minutes' conditioning time, then there would be three possible comparisons instead of one. For design and analysis, it is convenient to have a single standard against which the responses at all levels of all factors can be compared. In statistical methods the standard which has been adopted for ease and universality of reference is the mean value of the responses obtained for every test in an experiment.

In this report the response obtained for an individual test is represented by the letter  $y$  with appropriate subscripts representing the levels of the factors and the particular replication of the test. For example, let the conditioning time in the zinc flotation work be factor  $X_a$ , with levels  $k = 1, 2, 3$  corresponding to 2, 3, and 4 minutes of conditioning time, respectively. Let the replications of the experiment be  $r = 1, 2$ . The zinc recovery for 4 minutes' conditioning time and the second replicate is represented by  $y_{32}$ . In general, the zinc recovery for the  $k$ 'th level of conditioning time and the  $r$ 'th replicate is represented by  $y_{kr}$ . A bar above a symbol represents a mean value of the quantity represented by the symbol. The mean value of the two replicate flotation tests with 4 minutes' conditioning time is represented by  $\bar{y}_3$ , and the mean value for the  $k$ 'th level is represented by  $\bar{y}_k$ . The mean value of all observations in the experiment is represented by  $\bar{y}$ . The

difference between the average zinc recoveries at 4 minutes' conditioning time and the average of all the zinc recoveries is called the effect of conditioning time at the third level and is represented by  $\underline{A}_3$ . The effect of conditioning time at the third level is calculated as follows:

$$\underline{A}_3 = \bar{y}_3 - \bar{y}. \quad (12)$$

In general,

$$\underline{A}_k = \bar{y}_k - \bar{y}. \quad (13)$$

The letter A in the symbol  $\underline{A}_k$  is the capital of the letter a in the subscript of the symbol  $X_a$  representing conditioning time. With three levels of conditioning time the effects  $\underline{A}_k$  can be divided into linear components and quadratic components represented by  $A_k$  and  $A_k^2$ , respectively. This correlation of symbols for effects and symbols for factors is followed throughout this report.

The assumed true response function for the experiment is

$$Y = M_0 + M_a X_a + M_{aa} X_a^2. \quad (14)$$

The quantities  $A_k$  and  $A_k^2$  represent the components of the effect of factor  $X_a$  at the k'th level associated with the first and second powers of  $X_a$  in equation (14). In general, if there are p levels of a factor, it is possible to divide the effect of the factor into (p - 1) components. The fundamental nature of polynomial components and the basic procedures for calculating them now will be illustrated for linear, quadratic, and cubic components. Let the average values of the zinc recoveries at 2, 3, and 4 minutes' conditioning time be, respectively,  $\bar{y}_1 = 85$  percent,  $\bar{y}_2 = 89$  percent, and  $\bar{y}_3 = 91$  percent, with an average of  $\bar{y} = 88\frac{1}{3}$  percent.

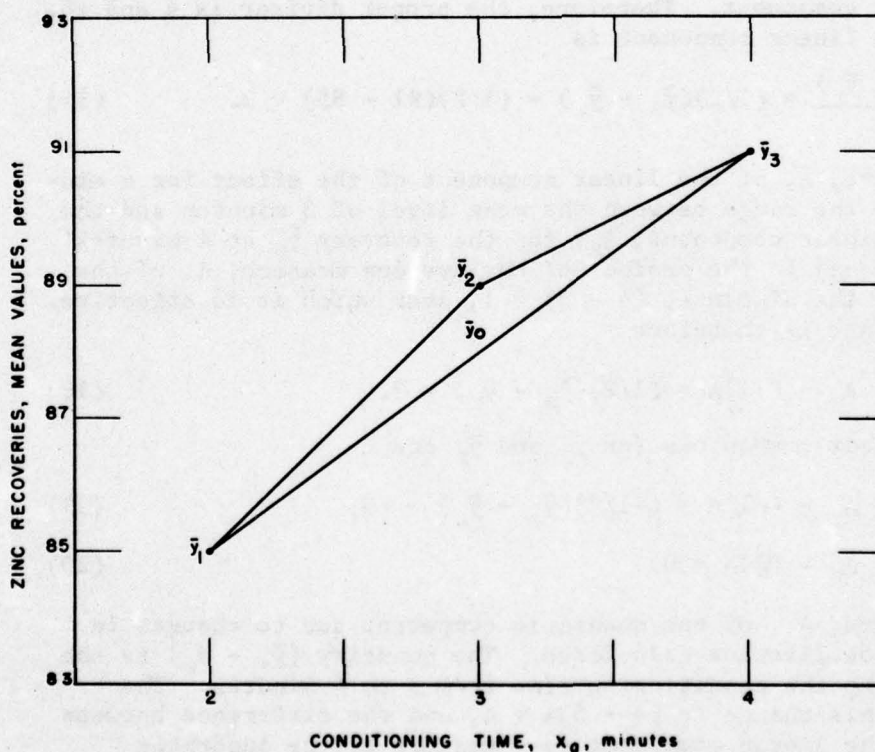


FIGURE 5. - Recovery Versus Conditioning Time in a Three-Level Experiment.



The determination of independent estimates of the polynomial components is accomplished by first shifting the factor origins to the center of the experiment from which the effects are measured. If the algebraic origin of the factor  $X_a$  is shifted from 0 to 3 minutes, the zinc recoveries then may be represented as shown in figure 5.

There are three ways of measuring linear changes in response due to changes in conditioning time, and these are indicated by the three lines joining the points in figure 5. The measures of the linear changes in response are  $\bar{y}_3 - \bar{y}_1$ ,  $\bar{y}_3 - \bar{y}_2$ , and  $\bar{y}_2 - \bar{y}_1$ . From these three measures of the linear component an average measure,  $A$ , of the linear component in the experiment can be obtained. The sum of these three quantities is

$$(\bar{y}_3 - \bar{y}_1) + (\bar{y}_3 - \bar{y}_2) + (\bar{y}_2 - \bar{y}_1) = 2\bar{y}_3 - 2\bar{y}_1 = 2(\bar{y}_3 - \bar{y}_1). \quad (15)$$

The proper divisor to obtain the average measure of the linear component needs to be ascertained. The quantity  $(\bar{y}_3 - \bar{y}_1)$  in equation (15) is equal to  $(\bar{y}_3 - \bar{y}_2) + (\bar{y}_2 - \bar{y}_1)$ . Therefore, equation (15) may be written

$$2(\bar{y}_3 - \bar{y}_2) + 2(\bar{y}_2 - \bar{y}_1) = 2(\bar{y}_3 - \bar{y}_1). \quad (16)$$

From equation (16) the quantity  $2(\bar{y}_3 - \bar{y}_1)$  is seen to be the sum of four basic measures of the linear component. Therefore, the proper divisor is 4 and the average measure of the linear component is

$$A = \frac{2(\bar{y}_3 - \bar{y}_1)}{4} = (1/2)(\bar{y}_3 - \bar{y}_1) = (1/2)(91 - 85) = 3. \quad (17)$$

The average measure,  $A$ , of the linear component of the effect for 4 minutes is effective over the range between the mean level of 3 minutes and the 4-minute level. The linear component,  $A_3$ , for the recovery  $\bar{y}_3$  at 4 minutes' conditioning time is equal to the product of the average measure,  $A$ , of the linear component times the distance,  $(4 - 3) = 1$ , over which it is effective. The linear component,  $A_3$ , is therefore

$$A_3 = (+1)A = (1/2)(\bar{y}_3 - \bar{y}_1) = 3. \quad (18)$$

In like manner the linear components for  $\bar{y}_1$  and  $\bar{y}_2$  are

$$A_1 = (-1)A = (-1/2)(\bar{y}_3 - \bar{y}_1) = -3, \quad (19)$$

$$A_2 = (0)A = 0. \quad (20)$$

The average measure,  $A^2$ , of the quadratic component due to changes in conditioning time can be likewise calculated. The quantity  $(\bar{y}_3 - \bar{y}_2)$  is the total effect of changing the conditioning time from 3 to 4 minutes. The linear component for this change is  $(4 - 3)A = A$ , and the difference between the total effect and the linear component is a measure of the quadratic component; that is,

$$(\bar{y}_3 - \bar{y}_2) - A = (\bar{y}_3 - \bar{y}_2) - (1/2)(\bar{y}_3 - \bar{y}_1) = (1/2)(\bar{y}_3 - 2\bar{y}_2 + \bar{y}_1). \quad (21)$$

Similarly a measure of the quadratic component is obtained for the difference between the recoveries  $\bar{y}_2$  and  $\bar{y}_1$ ; namely,

$$\begin{aligned} -[(\bar{y}_2 - \bar{y}_1) - A] &= -[(\bar{y}_2 - \bar{y}_1) - (1/2)(\bar{y}_3 - \bar{y}_1)] \\ &= (1/2)(\bar{y}_3 - 2\bar{y}_2 + \bar{y}_1). \end{aligned} \quad (22)$$

The average measure,  $A^2$ , of the quadratic component is the mean of the right-hand quantities in equations (21) and (22); that is,

$$A^2 = (1/2)(\bar{y}_3 - 2\bar{y}_2 + \bar{y}_1) = (1/2)[91 - 2(89) + 85] = -1. \quad (23)$$

Equation (23) may be rewritten as

$$A^2 = (1/2)(\bar{y}_3 - 2\bar{y}_2 + \bar{y}_1) = (1/2)[(\bar{y}_3 - \bar{y}_2) - (\bar{y}_2 - \bar{y}_1)]. \quad (24)$$

From equation (24) it is seen that the average measure of the quadratic component of the effect estimated from three equally spaced adjacent points of an experiment is equal to one-half the difference between the two adjacent measures of the linear component. In general, it may be said that the average measure of the quadratic component of the effect for three equally spaced values of the factor  $X_a$  is equal to the difference between the two adjacent basic measures of the linear component, calculated from pairs of adjacent points, divided by the number of factor units spanned by the three points.

It now is desirable to show the relationship between the average measure,  $A^2$ , of the quadratic component and the quadratic components  $A_1^2$ ,  $A_2^2$ , and  $A_3^2$  for the recoveries  $\bar{y}_1$ ,  $\bar{y}_2$ , and  $\bar{y}_3$ , respectively. From equation (12) the effect of conditioning time on the recovery  $\bar{y}_3$  is  $\underline{A}_3 = \bar{y}_3 - \bar{y}$ . The difference between the effect  $\underline{A}_3$  and the linear component,  $A_3$ , must be the quadratic component,  $A_3^2$ ; that is,

$$\begin{aligned} A_3^2 &= \underline{A}_3 - A_3 = (\bar{y}_3 - \bar{y}) - (1/2)(\bar{y}_3 - \bar{y}_1) \\ &= \bar{y}_3 - \frac{\bar{y}_1 + \bar{y}_2 + \bar{y}_3}{3} - (1/2)\bar{y}_3 + (1/2)\bar{y}_1 \\ &= (1/6)\bar{y}_3 - (2/6)\bar{y}_2 + (1/6)\bar{y}_1 = (1/3)(1/2)(\bar{y}_3 - 2\bar{y}_2 + \bar{y}_1) \\ &= (1/3)A^2 = (1/3)(-1) = -1/3. \end{aligned} \quad (25)$$

Similarly,

$$\begin{aligned} A_1^2 &= \underline{A}_1 - A_1 = (\bar{y}_1 - \bar{y}) - [(-1/2)(\bar{y}_3 - \bar{y}_1)] \\ &= \bar{y}_1 - \frac{\bar{y}_1 + \bar{y}_2 + \bar{y}_3}{3} + (1/2)\bar{y}_3 - (1/2)\bar{y}_1 \\ &= (1/3)(1/2)(\bar{y}_3 - 2\bar{y}_2 + \bar{y}_1) = (1/3)A^2 = -1/3; \end{aligned} \quad (26)$$

$$\begin{aligned} A_2^2 &= \underline{A}_2 - A_2 = (\bar{y}_2 - \bar{y}) - 0 = \bar{y}_2 - \frac{\bar{y}_1 + \bar{y}_2 + \bar{y}_3}{3} \\ &= (-2/3)(1/2)(\bar{y}_3 - 2\bar{y}_2 + \bar{y}_1) = (-2/3)A^2 \\ &= (-2/3)(-1) = 2/3. \end{aligned} \quad (27)$$

A numerical check on these calculations can be made by adding the linear and quadratic components for a particular recovery to the mean,  $\bar{y}$ . The result should be equal to the recovery; that is,

$$\bar{y}_k = \bar{y} + A_k + A_k^2 \quad (28)$$

For the third level of conditioning time,

$$\bar{y}_3 = \bar{y} + A_3 + A_3^2 = 88 - 1/3 + 3 + (-1/3) = 91$$

The average measures,  $A$  and  $A^2$ , of the linear and quadratic components, respectively, and these components in terms of  $A$  and  $A^2$  are listed for further reference:

$$\begin{aligned} A &= (1/2)(\bar{y}_3 - \bar{y}_1) \\ A^2 &= (1/2)(\bar{y}_3 - 2\bar{y}_2 + \bar{y}_1) \end{aligned} \quad (29)$$

$$\begin{aligned} A_1 &= (-1)A & A_1^2 &= (1/3)A^2 \\ A_2 &= (0)A & A_2^2 &= (-2/3)A^2 \\ A_3 &= (+1)A & A_3^2 &= (1/3)A^2 \end{aligned} \quad (30)$$

The investigation of the linear and quadratic components for a three-level experiment is relatively easy because of the simplicity of the design. The investigation of polynomial components for experiments with more than three levels requires a different approach. However, the development of the average measures of the polynomial components may be carried out on the basis of principles developed in the discussion of the three-level zinc flotation experiment.

Consider a zinc flotation experiment with all the tests given in the previous experiment and with two additional replicate tests with 5 minutes' conditioning time at the fourth level for which the average zinc recovery is 92 percent; that is,  $\bar{y}_1 = 85$ ;  $\bar{y}_2 = 89$ ;  $\bar{y}_3 = 91$ ;  $\bar{y}_4 = 92$ ; and  $\bar{y} = 89 - 1/4$ . The assumed true response function for the experiment is

$$Y = M_0 + M_a X_a + M_{aa} X_a^2 + M_{aaa} X_a^3 \quad (31)$$

The average measures,  $A$ ,  $A^2$ , and  $A^3$ , of the linear, quadratic, and cubic components, respectively, now must be calculated for the first, second, and third powers of  $X_a$  in equation (31).

The algebraic origin of the conditioning time,  $X_a$ , is first shifted from 0 to 3-1/2 minutes. The zinc recoveries then may be represented as shown in figure 6. There are six possible pairs of points which give measures of the linear component due to the changes in conditioning time shown in figure 6. These are



$$\begin{aligned}
\bar{y}_4 - \bar{y}_1 &= (\bar{y}_4 - \bar{y}_3) + (\bar{y}_3 - \bar{y}_2) + (\bar{y}_2 - \bar{y}_1), \\
\bar{y}_4 - \bar{y}_2 &= (\bar{y}_4 - \bar{y}_3) + (\bar{y}_3 - \bar{y}_2), \\
\bar{y}_4 - \bar{y}_3 &= (\bar{y}_4 - \bar{y}_3), \\
\bar{y}_3 - \bar{y}_1 &= (\bar{y}_3 - \bar{y}_2) + (\bar{y}_2 - \bar{y}_1), \\
\bar{y}_3 - \bar{y}_2 &= (\bar{y}_3 - \bar{y}_2), \\
\bar{y}_2 - \bar{y}_1 &= (\bar{y}_2 - \bar{y}_1).
\end{aligned} \tag{32}$$

The equations (32) show that the six pairs of points provide 10 basic measures,  $\bar{y}_k - \bar{y}_{k-1}$ , of the linear component. The average measure,  $A$ , of the linear component is

$$\begin{aligned}
A &= (1/10)(3\bar{y}_4 + \bar{y}_3 - \bar{y}_2 - 3\bar{y}_1) \\
&= (1/10)[3(92) + 91 - 89 - 3(85)] = 2-3/10.
\end{aligned} \tag{33}$$

As previously defined the difference between two adjacent measures of the linear component provided a measure of the quadratic component. Therefore, any two adjacent linear component measures in the group listed on the left side of equation (32) can be used to obtain a measure of the quadratic effect. If two adjacent linear component measures span unequal factor spaces, suitable weighting must be employed. For example, if the quadratic component were zero, the measure,  $\bar{y}_4 - \bar{y}_2$ , of the linear component would be twice as great as the adjacent measure,  $\bar{y}_3 - \bar{y}_1$ , of the linear component, whereas if the quadratic component were not zero, the quantity  $(\bar{y}_4 - \bar{y}_2) - 2(\bar{y}_3 - \bar{y}_1)$  would be its measure. There are four such measures of the quadratic component; that is,

$$\begin{aligned}
(\bar{y}_4 - \bar{y}_3) - (\bar{y}_3 - \bar{y}_2) &= (\bar{y}_4 - 2\bar{y}_3 + \bar{y}_2), \\
2(\bar{y}_4 - \bar{y}_3) - (\bar{y}_3 - \bar{y}_1) &= 2\bar{y}_4 - 3\bar{y}_3 + \bar{y}_1 \\
&= 2(\bar{y}_4 - 2\bar{y}_3 + \bar{y}_2) + (\bar{y}_3 - 2\bar{y}_2 + \bar{y}_1), \\
(\bar{y}_4 - \bar{y}_2) - 2(\bar{y}_3 - \bar{y}_1) &= \bar{y}_4 - 3\bar{y}_3 + 2\bar{y}_1 \\
&= (\bar{y}_4 - 2\bar{y}_3 + \bar{y}_2) + 2(\bar{y}_3 - 2\bar{y}_2 + \bar{y}_1), \\
(\bar{y}_3 - \bar{y}_2) - (\bar{y}_2 - \bar{y}_1) &= (\bar{y}_3 - 2\bar{y}_2 + \bar{y}_1).
\end{aligned} \tag{34}$$

From equations (23) and (24) in the case of the three-level zinc flotation experiment, it was seen that the quantity  $\bar{y}_3 - 2\bar{y}_2 + \bar{y}_1$  from three equally spaced adjacent points provides two basic measures of the quadratic component, just as two adjacent points provide one basic measure of the linear component. The 4 measures of the quadratic component on the left side of equation (34) provide 8 measures of the quadratic component in the form  $y_k - 2y_{k-1} + y_{k-2}$  for a total of 16 basic measures of the quadratic component. The sum of the effects in (34) is  $4\bar{y}_4 - 4\bar{y}_3 - 4\bar{y}_2 + 4\bar{y}_1$ , and the average measure,  $A^2$ , of the quadratic component is

$$\begin{aligned}
A^2 &= (1/16)(4\bar{y}_4 - 4\bar{y}_3 - 4\bar{y}_2 + 4\bar{y}_1) = (1/4)(\bar{y}_4 - \bar{y}_3 - \bar{y}_2 + \bar{y}_1) \\
&= (1/4)(92 - 91 - 89 + 85) = -3/4.
\end{aligned} \tag{35}$$

The discussion of equation set (34) reveals that the basic measures of the quadratic component are  $(1/2)(\bar{y}_4 - 2\bar{y}_3 + \bar{y}_2)$  and  $(1/2)(\bar{y}_3 - 2\bar{y}_2 + \bar{y}_1)$ . In general, for a three-level factor the average measure of the quadratic component is the difference between the two adjacent basic measures of the linear component divided by the number of factor units spanned by the measure of the quadratic component. Similarly, the average measure of the cubic component,  $A^3$ , for four levels is equal to the difference between the two adjacent basic measures of the quadratic component divided by the number of factor units spanned by the measure of the cubic component; that is,

$$\begin{aligned} A^3 &= (1/3)[(1/2)(\bar{y}_4 - 2\bar{y}_3 + \bar{y}_2) - (1/2)(\bar{y}_3 - 2\bar{y}_2 + \bar{y}_1)] \\ &= (1/6)(\bar{y}_4 - 3\bar{y}_3 + 3\bar{y}_2 - \bar{y}_1) \\ &= (1/6)[92 - 3(91) + 3(89) - 85] = 1/6. \end{aligned} \quad (36)$$

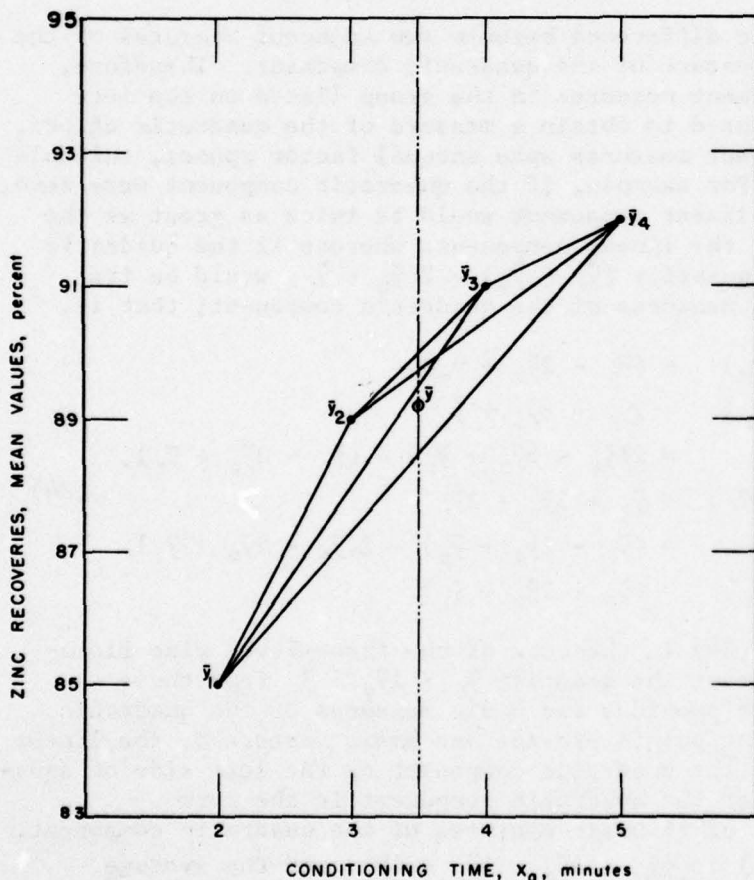


FIGURE 6. - Recovery Versus Conditioning Time in a Four-Level Experiment.

It now is desirable to determine the relationship between the polynomial components  $A_k$ ,  $A_k^2$ , and  $A_k^3$  and the corresponding average measures of such components. A knowledge of this relationship makes it possible to calculate the polynomial components. These polynomial components are related to the average recovery at the  $k$ 'th level of conditioning time as follows:

$$\begin{aligned} \bar{y}_k &= \bar{y} + A_k = \bar{y} + A_k \\ &\quad + A_k^2 + A_k^3. \end{aligned} \quad (37)$$

There are functions of  $X$ , that, when multiplied by the average measures,  $A$ ,  $A^2$ , and  $A^3$ , will give the corresponding linear, quadratic, and cubic components shown in equation (37). Let these functions be  $Z_{1k}$ ,  $Z_{2k}$ , and  $Z_{3k}$  such that the following relationships hold true:

$$\begin{aligned}
A_k &= AZ_1 k, \\
A_k^2 &= A^2 Z_2 k, \\
A_k^3 &= A^3 Z_3 k.
\end{aligned} \tag{38}$$

From equations (37) and (38) we now obtain

$$\bar{y}_k = \bar{y} + AZ_1 k + A^2 Z_2 k + A^3 Z_3 k. \tag{39}$$

In a more general way the response function in equation (39) may be written

$$y = \bar{y} + AZ_1 + A^2 Z_2 + A^3 Z_3. \tag{40}$$

The determination of the functions  $Z_1$ ,  $Z_2$ , and  $Z_3$  can be accomplished by an investigation of the estimated response function for equation (31); that is,

$$y = m_0 + m_a X_a + m_{aa} X_a^2 + m_{aaa} X_a^3. \tag{41}$$

The first step in the investigation is to transform equation (41) so that it is expressed in terms of a new independent variable with its origin at the midpoint of the range of the conditioning time,  $X_a$ . The transformation  $X_a = X'_a + 7/2$  will make  $X'_a = X_a - 7/2$  the new independent variable with origin at  $X_a = 7/2$  as shown in figure 6. The substitution of  $X_a = X'_a + 7/2$  in equation (41) makes it possible to write the response function as

$$y = p_0 + p_a X'_a + p_{aa} X_a'^2 + p_{aaa} X_a'^3, \tag{42}$$

$$y = p_0 + p_a (X_a - 7/2) + p_{aa} (X_a - 7/2)^2 + p_{aaa} (X_a - 7/2)^3. \tag{43}$$

The  $p_i$  in equations (42) and (43) are functions of the  $m_i$  in equation (41), which are determined when like powers of  $X'_a$  are collected after the original substitution.

From equation (43) and the individual zinc recoveries we obtain the general relationship,

$$\bar{y}_k = p_0 + p_a (X_a - 7/2)_k + p_{aa} (X_a - 7/2)_k^2 + p_{aaa} (X_a - 7/2)_k^3. \tag{44}$$

From equation (44) and the values of  $(X_a - 7/2)_k$  shown in figure 6 we obtain

$$\begin{aligned}
\bar{y}_1 &= p_0 - (3/2)p_a + (9/4)p_{aa} - (27/8)p_{aaa}, \\
\bar{y}_2 &= p_0 - (1/2)p_a + (1/4)p_{aa} - (1/8)p_{aaa}, \\
\bar{y}_3 &= p_0 + (1/2)p_a + (1/4)p_{aa} + (1/8)p_{aaa}, \\
\bar{y}_4 &= p_0 + (3/2)p_a + (9/4)p_{aa} + (27/8)p_{aaa}.
\end{aligned} \tag{45}$$



The sum of the equations (45) is,  $\sum_k \bar{y}_k = 4p_0 + (20/4)p_{aa}$ , and the mean,  $\bar{y}$ , is

$$\bar{y} = p_0 + (5/4)p_{aa}. \quad (46)$$

From equations (33) and (45) we obtain

$$\begin{aligned} A &= (1/10)(3\bar{y}_4 + \bar{y}_3 - \bar{y}_2 - 3\bar{y}_1) \\ &= (1/10)[3p_0 + (9/2)p_a + (27/4)p_{aa} + (81/8)p_{aaa} \\ &\quad + p_0 + (1/2)p_a + (1/4)p_{aa} + (1/8)p_{aaa} \\ &\quad - p_0 + (1/2)p_a - (1/4)p_{aa} + (1/8)p_{aaa} \\ &\quad - 3p_0 + (9/2)p_a - (27/4)p_{aa} + (81/8)p_{aaa}] \\ &= (1/10)[10p_a + (41/2)p_{aaa}] = p_a + (41/20)p_{aaa}. \end{aligned} \quad (47)$$

In a similar way we obtain from equations (35), (36), and (45)

$$A^2 = (1/4)(\bar{y}_4 - \bar{y}_3 - \bar{y}_2 + \bar{y}_1) = p_{aa}, \quad (48)$$

$$A^3 = (1/6)(\bar{y}_4 - 3\bar{y}_3 + 3\bar{y}_2 - \bar{y}_1) = p_{aaa}. \quad (49)$$

From equations (43), (46), (47), (48), and (49) we obtain the relationship,

$$\begin{aligned} y &= [\bar{y} - (5/4)A^2] + [A - (41/20)A^3](X_a - 7/2) \\ &\quad + A^2(X_a - 7/2)^2 + A^3(X_a - 7/2)^3 \\ &= \bar{y} + A(X_a - 7/2) + A^2[(X_a - 7/2)^2 - 5/4] \\ &\quad + A^3[(X_a - 7/2)^3 - (41/20)(X_a - 7/2)]. \end{aligned} \quad (50)$$

A comparison of equations (40) and (50) shows that

$$\begin{aligned} Z_1 &= (X_a - 7/2), \\ Z_2 &= (X_a - 7/2)^2 - 5/4, \\ Z_3 &= (X_a - 7/2)^3 - (41/20)(X_a - 7/2). \end{aligned} \quad (51)$$

The functions  $Z_1$ ,  $Z_2$ , and  $Z_3$  have been shown to be polynomials in  $X_a$ . For the  $k$ 'th level of conditioning time,

$$\begin{aligned} Z_{1k} &= (X_a - 7/2)_k, \\ Z_{2k} &= (X_a - 7/2)_k^2 - 5/4, \\ Z_{3k} &= (X_a - 7/2)_k^3 - (41/20)(X_a - 7/2)_k. \end{aligned} \quad (52)$$

Equations (52) and the values of  $(X_a - 7/2)_k$  from figure 6 give

$$\begin{aligned}
 Z_{11} &= -3/2, \\
 Z_{12} &= -1/2, \\
 Z_{13} &= +1/2, \\
 Z_{14} &= +3/2, \\
 Z_{21} &= (-3/2)^2 - 5/4 = +1, \\
 Z_{22} &= (-1/2)^2 - 5/4 = -1, \\
 Z_{23} &= (+1/2)^2 - 5/4 = -1, \\
 Z_{24} &= (+3/2)^2 - 5/4 = +1, \\
 Z_{31} &= (-3/2)^3 - (41/20)(-3/2) = -3/10, \\
 Z_{32} &= (-1/2)^3 - (41/20)(-1/2) = +9/10, \\
 Z_{33} &= (+1/2)^3 - (41/20)(+1/2) = -9/10, \\
 Z_{34} &= (+3/2)^3 - (41/20)(+3/2) = +3/10.
 \end{aligned} \tag{53}$$

From equations (33), (35), (36), (38), and (53) the values of the polynomial components are calculated as

$$\begin{aligned}
 A_1 &= AZ_{11} = (23/10)(-3/2) = -69/20, \\
 A_2 &= AZ_{12} = (23/10)(-1/2) = -23/20, \\
 A_3 &= AZ_{13} = (23/10)(1/2) = +23/20, \\
 A_4 &= AZ_{14} = (23/10)(3/2) = +69/20, \\
 A_1^2 &= A^2 Z_{21} = (-3/4)(1) = -3/4, \\
 A_2^2 &= A^2 Z_{22} = (-3/4)(-1) = 3/4, \\
 A_3^2 &= A^2 Z_{23} = (-3/4)(-1) = 3/4, \\
 A_4^2 &= A^2 Z_{24} = (-3/4)(1) = -3/4, \\
 A_1^3 &= A^3 Z_{31} = (1/6)(-3/10) = -1/20, \\
 A_2^3 &= A^3 Z_{32} = (1/6)(9/10) = 3/20, \\
 A_3^3 &= A^3 Z_{33} = (1/6)(-9/10) = -3/20, \\
 A_4^3 &= A^3 Z_{34} = (1/6)(3/10) = 1/20.
 \end{aligned} \tag{54}$$

A numerical check on these calculations can be made by adding the linear, quadratic, and cubic components for a particular recovery to the mean,  $\bar{y}$ . The result should be equal to the recovery; namely,

$$\begin{aligned}\bar{y}_3 &= \bar{y} + A_3 + A_3^2 + A_3^3 \\ &= 89-1/4 + 23/20 + 3/4 + (-3/20) = 91.\end{aligned}$$

The determination of these polynomial components permits the examination of their importance from level to level in an experiment and the analysis of their importance as compared to the experimental error and to one another. The evaluation of their importance serves as a guide to further design of experiments.

#### Orthogonal Transformation of Response Functions

There is a mathematical transformation of a response function for experiments with evenly spaced factor levels that facilitates the investigation of factor effects and their polynomial components and makes it possible to design experiments so that the investigation may be concluded with a minimum of work in designs, experiments, and analyses of data. Furthermore, the use of the principles that underlie the transformation yields more satisfactory, comprehensive, and conclusive information about the relationships involved in many research problems. The transformation is called orthogonal because it changes the form of the response function so that the terms of the response function form a set of orthogonal polynomials in the factors involved and the coefficients of the terms form a set of orthogonal polynomials in the observations of the experiment. Orthogonality is basically a mathematical concept of two or more functions which can be graphed as vectors crossing each other at right angles. A discussion of orthogonality, with examples, is presented next before proceeding to the detailed development of orthogonal transformations.

The development of the polynomial components and the average measures of the polynomial components involves the fundamental principles underlying the orthogonal transformation to be discussed. The zinc recovery was the response and the conditioning time was factor  $X_a$ , with levels  $k = 1, 2, 3, 4$  corresponding to 2, 3, 4, and 5 minutes. The estimated response function for the experiment was shown in equation (41), as follows:

$$y = m_0 + m_a X_a + m_{aa} X_a^2 + m_{aaa} X_a^3.$$

The transformed equation was shown in equation (40) to be

$$\begin{aligned}y &= \bar{y} + AZ_1 + A^2 Z_2 + A^3 Z_3, \\ A &= (1/10)(3\bar{y}_4 + \bar{y}_3 - \bar{y}_2 - 3\bar{y}_1), \\ A^2 &= (1/4)(\bar{y}_4 - \bar{y}_3 - \bar{y}_2 + \bar{y}_1), \\ A^3 &= (1/6)(\bar{y}_4 - 3\bar{y}_3 + 3\bar{y}_2 - \bar{y}_1), \\ Z_1 &= (X_a - 7/2), \\ Z_2 &= (X_a - 7/2)^2 - 5/4, \\ Z_3 &= (X_a - 7/2)^3 - (41/20)(X_a - 7/2).\end{aligned}\tag{55}$$



The average measures,  $A$ ,  $A^2$ , and  $A^3$  of the linear, quadratic, and cubic effects, are coefficients of the  $Z$  polynomials and are hereafter referred to as the linear, quadratic, and cubic coefficients of the corresponding polynomial components of the effect of factor  $X_a$ . These coefficients are orthogonal polynomials in the observations  $\bar{y}_k$ . The coefficients are called orthogonal because the sum of the products of the coefficients of the corresponding observations is zero. For example, consider the coefficients  $A^2$  and  $A^3$  in equation set (55):

$$A^2 = (1/4)\bar{y}_4 - (1/4)\bar{y}_3 - (1/4)\bar{y}_2 + (1/4)\bar{y}_1,$$

$$A^3 = (1/6)\bar{y}_4 - (3/6)\bar{y}_3 + (3/6)\bar{y}_2 - (1/6)\bar{y}_1.$$

The sum of the products of the corresponding coefficients of the  $\bar{y}_k$  is

$$(1/4)(1/6) + (-1/4)(-3/6) + (-1/4)(3/6) + (1/4)(-1/6) = 0.$$

It later will be shown that the coefficients of the observations in equation (55) are simple multiples of the  $Z$  polynomials. The sum of the products of the corresponding coefficients of the  $\bar{y}_k$  is zero because it contains the factor  $\sum_k Z_{2k} Z_{3k} = 0$ . The  $Z_i$  in equation set (51) also are called orthogonal polynomials because the  $Z_{ik}$  shown in equation set (53) have the property that  $\sum_k Z_{ik} Z_{tk} = 0$ ;  $i \neq t$ ;  $i$ , and  $t = 1, 2, 3$ ; for example,

$$\sum_k Z_{2k} Z_{3k} = (+1)(-3/10) + (-1)(+9/10) + (-1)(-9/10) + (+1)(+3/10) = 0.$$

It would be undesirable to develop polynomial components and their coefficients in the laborious manner of the preceding section. Fortunately, the principles underlying the orthogonal transformation make possible the development of a comprehensive system for the calculation of the orthogonal coefficients and the separation of the polynomial components with relative ease, however complex the problem may be.

#### Transformation of One-Factor Response Functions

To construct a comprehensive system for experimental design and analysis of the components of complex response functions, it is necessary to start from simple and easily understood principles. These will be developed by detailed discussion and illustration of the orthogonal transformation of one-factor response functions. For an experiment involving one factor,  $X_a$ , with evenly spaced levels  $k = 1, \dots, n$  and with replicates  $r = 1, \dots, q$ , the assumed true response function is

$$Y = M_0 + M_a X_a + M_{aa} X_a^2 + \dots + M_{aa\dots a} X_a^{n-1}. \quad (56)$$

As previously discussed, it is convenient to use the central values of the response and the factor range in an experiment for the evaluation of responses and the measurement of effects. If  $w$  represents the spacing between levels of factor  $X_a$ , the origin of factor  $X_a$  can be shifted to the center of the experiment with a change in factor units by the transformation

$$z = \frac{X_a - \bar{X}_a}{w} \quad (57)$$

For the factor levels  $k = 1, 2, \dots, n$ , the center of the  $n$  levels is  $\frac{n+1}{2}$ . The relationship between  $z$  and  $k$  then will be

$$z_k = k - \frac{n+1}{2}, \quad (58)$$

and specifically,

$$\begin{aligned} z_1 &= -\frac{n-1}{2}, \\ z_2 &= -\frac{n-3}{2}, \\ &\dots\dots\dots, \\ z_{n-1} &= \frac{n-3}{2}, \\ z_n &= \frac{n-1}{2}. \end{aligned} \quad (59)$$

If  $n$  is odd the values of  $z$  will be integers, and if  $n$  is even the values of  $z$  will be odd multiples of  $1/2$ .

This shift in the factor origin makes it possible to write the true response function in the form

$$Y = N_0 + N_1 z + N_2 z^2 + \dots + N_{n-1} z^{n-1}. \quad (60)$$

The  $N_i$ ,  $i = 0, 1, 2, \dots, (n-1)$ , in equation (60) are determined by collecting terms with like powers of  $z$  when the substitution  $X_a = wz + \bar{X}_a$  is made in equation (56). If  $\phi_1 Z_1$  were the linear component of the true effect of  $X_a$  and in general  $\phi_i Z_i$  were the  $i$ 'th polynomial component of the true effect of factor  $X_a$  corresponding to the successive  $i$ 'th powers of  $X_a$  in equation (56), the true response function may be expressed in the form

$$Y = \phi_0 Z_0 + \phi_1 Z_1 + \phi_2 Z_2 + \dots + \phi_{n-1} Z_{n-1}. \quad (61)$$

The separation of the true effect of factor  $X_a$  into the independent components  $\phi_1 Z_1, \dots, \phi_{n-1} Z_{n-1}$  can be accomplished if the  $Z_i$  are orthogonal polynomials in the variable  $z = (X_a - \bar{X}_a)/w$  of equation (60). The condition of orthogonality of the  $Z_i$  insures the independence of the terms  $\phi_i Z_i$ . The response function in equation (61) is the orthogonal transformation of the response function shown in equation (56).

The  $\phi_i$  of equation (61) can be estimated from the observations obtained when the experiment is performed. The estimated response function then will be of the form

$$y = A^0 Z_0 + A^1 Z_1 + A^2 Z_2 + \dots + A^{n-1} Z_{n-1}. \quad (62)$$

Equation (62) is similar in form to equation (40) which was obtained in the previous discussion of the four-level single-factor zinc flotation experiment. The  $A^i$  of equation (62) are estimates of the  $\phi_i$  of equation (61) and can be

calculated in terms of the values of  $Z_i$  at the factor levels. In the general case of response functions with the form

$$M_0 X^0 + M_1 X + M_2 X^2 + \dots + M_{n-1} X^{n-1} \quad (63)$$

for  $n$  equally spaced values,  $X = 0, 1, 2, \dots, (n-1)$ , the derivation of orthogonal polynomials,  $P_i$ , has been shown by Kendall<sup>5</sup> and is explicitly shown for  $P_1, P_2, \dots, P_6$ ;  $P_0 = 1$ . For the variable  $z$  in equation (60) the orthogonal polynomials,  $Z_i$ , of equations (61) and (62) can be calculated from Kendall's  $P_i$  by the substitution  $X = z + (n-1)/2$ . The results are as follows:

$$\begin{aligned} Z_0 &= 1, \\ Z_1 &= z, \\ Z_2 &= z^2 - \frac{n^2 - 1}{12}, \\ Z_3 &= z^3 - \left[ \frac{3n^2 - 7}{20} \right] z, \\ Z_4 &= z^4 - \left[ \frac{3n^2 - 13}{14} \right] z^2 + \frac{3(n^2 - 1)(n^2 - 9)}{560}, \\ Z_5 &= z^5 - \left[ \frac{5(n^2 - 7)}{18} \right] z^3 + \left[ \frac{15n^4 - 230n^2 + 407}{1008} \right] z, \\ Z_6 &= z^6 - \left[ \frac{5(3n^2 - 31)}{44} \right] z^4 + \left[ \frac{5n^4 - 110n^2 + 329}{176} \right] z^2 \\ &\quad - \frac{5(n^2 - 1)(n^2 - 9)(n^2 - 25)}{14784}. \end{aligned} \quad (64)$$

If  $z = (X_a - 7/2)$  and  $n = 4$ , the resulting polynomials  $Z_1, Z_2$ , and  $Z_3$  are the same as previously shown in equation set (51) for the four-level zinc flotation experiment. Bennett and Franklin<sup>6</sup> have given a recursion formula by means of which the value of any  $i$ 'th  $Z$  polynomial may be calculated from the values of  $Z_{i-1}$ ,  $Z_{i-2}$ , and  $Z_1$ . In the terminology of this paper the formula is

$$Z_i = Z_{i-1} Z_1 - \left[ \frac{(i-1)^2 [n^2 - (i-1)^2]}{4 [4(i-1)^2 - 1]} \right] Z_{i-2}. \quad (65)$$

Since equations for the  $Z_i$  polynomials have been established, it now is possible to obtain a general solution for the  $A^i$  in terms of the corresponding  $Z_{ik}$  where the  $Z_{ik}$  are the values of  $Z_i$  at the  $k$ 'th level. For the  $k$ 'th level of factor  $X_a$  the general relationship of equation (62) becomes

$$\bar{y}_k = A^0 Z_{0k} + A Z_{1k} + A^2 Z_{2k} + \dots + A^{n-1} Z_{(n-1)k}. \quad (66)$$

<sup>5</sup>Kendall, M. G., *The Advanced Theory of Statistics*: Hafner Publishing Co., New York, N.Y., vol. 2, 3d ed., 1951, pp. 159-161.

<sup>6</sup>Bennett, C. A., and Franklin, N. L., *Statistical Analysis in Chemistry and the Chemical Industry*: John Wiley & Sons, Inc., New York, N.Y., 1954, p. 257.



The values of the  $Z_{ik}$  of equation (66) are determined from equation set (64) for the values of  $z = z_k$  at the  $k$ 'th level. There are  $n$  equations of the type of equation (66) in  $n$  unknowns  $A^0, A, A^2, \dots, A^{n-1}$ . The  $A^i$  can, therefore, be resolved in terms of the  $Z_{ik}$ , and the resulting general formula for the  $A^i$  is

$$A^i = \frac{\sum_k Z_{ik} \bar{y}_k}{\sum_k Z_{ik}^2} = \frac{\sum_{kr} Z_{ik} y_{kr}}{Q \sum_k Z_{ik}^2}. \quad (67)$$

From equation set (64)  $Z_{0k} = Z_0 = 1$  and the solution for  $A^0$  is

$$A^0 = \frac{\sum_k \bar{y}_k}{\sum_k (1)^2} = \bar{y}. \quad (68)$$

From equation (68) the first term in equation (62) is  $A^0 Z_0 = \bar{y}(1) = \bar{y}$ , which is the same as the first term in the response function of equation (40) for the single-factor zinc flotation experiment previously discussed. Equation (62) then may be written

$$y = \bar{y} + A Z_1 + A^2 Z_2 + \dots + A^{n-1} Z_{n-1}. \quad (69)$$

By means of the relationships in equations (57) and (64), equation (69) may be converted to the form

$$y = m_0 + m_a X_a + m_{aa} X_a^2 + \dots + m_{aa \dots a} X_a^{n-1}. \quad (70)$$

The coefficients in equation (70) are estimates of the corresponding coefficients in the true response function of equation (56).

The values of the  $Z_{ik}$  frequently are fractional, and all contain a common factor for a particular  $Z_i$  and a particular value of  $n$ . Values of  $Z'_{ik}$  other than  $Z'_{0k}$  have been extensively tabulated by Fisher and Yates<sup>7</sup> for the set of smallest possible integral values of  $Z_{ik}$  such that  $Z_{ik} = W_i Z'_{ik}$  and  $W_i =$  a constant. Substitution of  $Z_{ik} = Z'_{ik}/W_i$  in equation (67) gives an expression for the  $A^i$  in terms of the  $Z'_{ik}$ ; that is,

$$A^i = \sum_{kr} (Z'_{ik}/W_i) y_{kr} / Q \sum_k (Z'_{ik}/W_i)^2 = W_i \sum_{kr} Z'_{ik} y_{kr} / Q \sum_k Z_{ik}^2. \quad (71)$$

In this report the quantities  $\sum_{kr} Z'_{ik} y_{kr}$  and  $\sum_k Z_{ik}^2$  are represented by  $\phi_i$  and  $Q_i$ , respectively. Equation (71) then may be written

$$A^i = (W_i / Q_i) \phi_i. \quad (72)$$

The values of  $W_i$  and  $Q_i$  are common to all  $Z'_{ik}$  for a particular value of  $n$  and a particular value of  $i$ . Values of  $W_i$  and  $Q_i$  also are tabulated with the values of the  $Z'_{ik}$ . The values of  $Z'_{ik}$ ,  $W_i$ , and  $Q_i$  for small values of  $n$  may be easily determined from equation set (64) by use of the relationships discussed here. Values of  $Z'_{ik}$ ,  $W_i$ , and  $Q_i$  for values of  $n = 2, 3, 4$ , and  $5$  are shown in table 1.

<sup>7</sup>Fisher, R. A., and Yates, F., Statistical Tables for Biological, Agricultural, and Medical Research: Hafner Publishing Co., Inc., New York, N.Y., 1957, pp. 90-100.

TABLE 1. - Numerical values for the mean, linear, quadratic, cubic, and quartic orthogonal polynomials

Design level value of z	n = 2		n = 3			n = 4				n = 5				
	Z'ok	Z'1k	Z'ok	Z'1k	Z'2k	Z'ok	Z'1k	Z'2k	Z'3k	Z'ok	Z'1k	Z'2k	Z'3k	Z'4k <sup>1</sup>
-2						+1	-3	+1	-1	+1	-2	+2	-1	+1
-1			+1	-1	+1	+1	-1	-1	+3	+1	-1	-1	+2	-4
0	+1	-1	+1	0	-2	+1	+1	-1	-3	+1	0	-2	0	+6
+1	+1	+1	+1	+1	+1	+1	+1	-1	-3	+1	+1	-1	-2	-4
+2						+1	+3	+1	+1	+1	+2	+2	+1	+1
Q <sub>1</sub>	2	2	3	2	6	4	20	4	20	5	10	14	10	70
W <sub>1</sub>	1	2	1	1	3	1	2	1	10/3	1	1	1	5/6	35/12

<sup>1</sup>The factor level k = 1, 2, 3, 4, 5 is counted from the top for any particular Z'ik. Values for the mean, linear, quadratic, cubic, and quartic orthogonal polynomials are Z'ok, Z'1k, Z'2k, Z'3k, and Z'4k, respectively.

The Z'1k for n = 2 shown in table 1 usually are not published because of the simplicity of a one-factor experiment at two levels. The Z'1k for n = 2 and all Z'ok have been included in table 1 in order to facilitate the explanation of how to separate the polynomial components when more than one factor is involved. The inclusion of these features in the table makes possible a comprehensive notation which is helpful. A characteristic of the Z'ik and the Z'1k except Z'ok and Z'ok for all values of n is that

$$\sum_k Z'_{ik} = \sum_k Z'_{1k} = 0. \quad (73)$$

This characteristic is helpful in later developments and may be observed for the Z'1k in table 1.

The calculation of the polynomial coefficients A, A<sup>2</sup>, and A<sup>3</sup> according to equation (72) now will be demonstrated for the case of the four-level zinc flotation experiment previously discussed, and the quantities will be compared with those previously obtained and listed in equation set (55). For this purpose equation (72) may be modified to give a function in terms of the mean observations  $\bar{y}_k$  as follows:

$$\begin{aligned} A^1 &= (W_1/qQ_1)\phi_1 = (W_1/qQ_1)\sum_{kr} Z'_{1k} y_{kr} = (W_1/qQ_1)\sum_k Z'_{1k} \sum_r y_{kr} \\ &= (W_1/Q_1)\sum_k Z'_{1k} (\sum_r y_{kr}/q) = (W_1/Q_1)\sum_k Z'_{1k} \bar{y}_k. \end{aligned} \quad (74)$$



By means of equation (74) the coefficients  $A$ ,  $A^2$ , and  $A^3$  then may be expressed as

$$\begin{aligned} A &= (W_1/Q_1) \sum_k Z'_{1k} \bar{y}_k = (W_1/Q_1) (Z'_{11} \bar{y}_1 + Z'_{12} \bar{y}_2 + Z'_{13} \bar{y}_3 + Z'_{14} \bar{y}_4), \\ A^2 &= (W_2/Q_2) \sum_k Z'_{2k} \bar{y}_k = (W_2/Q_2) (Z'_{21} \bar{y}_1 + Z'_{22} \bar{y}_2 + Z'_{23} \bar{y}_3 + Z'_{24} \bar{y}_4), \\ A^3 &= (W_3/Q_3) \sum_k Z'_{3k} \bar{y}_k = (W_3/Q_3) (Z'_{31} \bar{y}_1 + Z'_{32} \bar{y}_2 + Z'_{33} \bar{y}_3 + Z'_{34} \bar{y}_4). \end{aligned} \quad (75)$$

By using the values of  $Z'_{ik}$ ,  $W_i$ , and  $Q_i$  as shown in table 1 for  $n = 4$ , the values of  $A$ ,  $A^2$ , and  $A^3$  in equation set (75) are shown to be

$$\begin{aligned} A &= (2/20)(-3\bar{y}_1 - \bar{y}_2 + \bar{y}_3 + 3\bar{y}_4), \\ A^2 &= (1/4)(\bar{y}_1 - \bar{y}_2 - \bar{y}_3 + \bar{y}_4), \\ A^3 &= [(10/3)/20](-\bar{y}_1 + 3\bar{y}_2 - 3\bar{y}_3 + \bar{y}_4). \end{aligned} \quad (76)$$

A comparison of the quantities in equation set (76) with those in equation set (55) will show that they are identical. It thus has been demonstrated that the values of the polynomial coefficients calculated on the basis of equation (72) are the same as those previously obtained by laborious analysis of the effects.

#### Transformation of Two-Factor Response Functions

The usefulness of the results obtained in the orthogonal transformation of a one-factor response function for a similar transformation of a two-factor response function now will be demonstrated. A generalization then will be made for response functions containing more than two factors.

Consider an experiment in the flotation of manganese in which the true manganese recovery is the true response,  $Y$ , and the factors are conditioning time represented by  $X_a$  and temperature represented by  $X_b$ . Let the number of replicates be  $r = 1, \dots, q$ , and specifically let  $r = 1, 2$ . Let the levels of  $X_a$  be  $k = 1, 2, 3$ , corresponding to 3, 4, and 5 minutes' conditioning time, respectively, and let the levels of  $X_b$  be  $m = 1, 2, 3, 4$ , corresponding to 30°, 40°, 50°, and 60° C., respectively. The manganese recovery for 5 minutes' conditioning time, a temperature of 40° C., and the first replicate of the test is denoted by  $y_{321}$ . In general the manganese recovery for the  $k$ 'th level of conditioning time, the  $m$ 'th level of temperature, and the  $r$ 'th replicate is  $y_{kmr}$ . The corresponding sum of replicate recoveries is  $y_{km} = \sum_r y_{kmr}$ , and the corresponding average manganese recovery is  $\bar{y}_{km}$ . Let the sums of replicate recoveries be as shown in the array (77) and the corresponding average manganese recoveries as shown in the array (78).

$$\begin{aligned} y_{11} &= 154.0 & y_{12} &= 156.0 & y_{13} &= 158.0 & y_{14} &= 160.0 \\ y_{21} &= 158.0 & y_{22} &= 162.0 & y_{23} &= 164.0 & y_{24} &= 166.0 \\ y_{31} &= 160.0 & y_{32} &= 164.0 & y_{33} &= 168.0 & y_{34} &= 170.0 \end{aligned} \quad (77)$$

$$\begin{aligned}
\bar{y}_{11} &= 77.0 & \bar{y}_{12} &= 78.0 & \bar{y}_{13} &= 79.0 & \bar{y}_{14} &= 80.0 \\
\bar{y}_{21} &= 79.0 & \bar{y}_{22} &= 81.0 & \bar{y}_{23} &= 82.0 & \bar{y}_{24} &= 83.0 \\
\bar{y}_{31} &= 80.0 & \bar{y}_{32} &= 82.0 & \bar{y}_{33} &= 84.0 & \bar{y}_{34} &= 85.0 \\
\bar{y} &= 80-5/6
\end{aligned} \tag{78}$$

The assumed true response function for the experiment is

$$\begin{aligned}
Y = & M_0 + M_a X_a + M_b X_b + M_{aa} X_a^2 + M_{bb} X_b^2 + M_{bbb} X_b^3 + M_{ab} X_a X_b \\
& + M_{abb} X_a X_b^2 + M_{abbb} X_a X_b^3 + M_{aab} X_a^2 X_b + M_{aabb} X_a^2 X_b^2 \\
& + M_{aabbb} X_a^2 X_b^3.
\end{aligned} \tag{79}$$

In equation (79) the product variables  $X_a X_b, X_a X_b^2$ , etc., are included in order to account for the mutual influence which the two factors have upon each other in affecting the manganese recoveries. This mutual influence is called an interaction, and the interaction effects may be evaluated separately from the main effects of conditioning time and temperature. If  $w_a$  were the spacing between levels of conditioning time and  $w_b$  were the spacing between levels of temperature, the origin for the two factors  $X_a$  and  $X_b$  can be shifted to the center of the experiment with a change in factor units by the transformations

$$\begin{aligned}
z_a &= \frac{X_a - \bar{X}_a}{w_a} = \frac{X_a - 4}{1} = X_a - 4, \\
z_b &= \frac{X_b - \bar{X}_b}{w_b} = \frac{X_b - 45}{10}.
\end{aligned} \tag{80}$$

This shift in factor origin makes it possible to write the true response function in the form

$$\begin{aligned}
Y = & N_{00} + N_{10} z_a + N_{01} z_b + N_{20} z_a^2 + N_{02} z_b^2 + N_{03} z_b^3 + N_{11} z_a z_b \\
& + N_{12} z_a z_b^2 + N_{13} z_a z_b^3 + N_{21} z_a^2 z_b + N_{22} z_a^2 z_b^2 \\
& + N_{23} z_a^2 z_b^3.
\end{aligned} \tag{81}$$

The  $N_{ij}$  of equation (81) are constants with subscripts corresponding to the powers of  $z_a^i$  and  $z_b^j$ . As for a one-factor experiment, equation (81) can be orthogonally transformed into the equation

$$\begin{aligned}
Y = & \phi_{00} Z_{00} + \phi_{10} Z_{10} + \phi_{01} Z_{01} + \phi_{20} Z_{20} + \phi_{02} Z_{02} + \phi_{03} Z_{03} \\
& + \phi_{11} Z_{11} + \phi_{12} Z_{12} + \phi_{13} Z_{13} + \phi_{21} Z_{21} + \phi_{22} Z_{22} + \phi_{23} Z_{23}.
\end{aligned} \tag{82}$$

The  $Z_{ij}$  are orthogonal polynomials of the  $i$ 'th degree in  $z_a$  and of the  $j$ 'th degree in  $z_b$ . The  $Z_{ij}$  are the products of the corresponding  $Z_i$  and  $Z_j$  for one-factor transformations. For example,  $Z_{13} = Z_1 Z_3$  where  $Z_1$  is the first degree orthogonal polynomial in  $z_a$ , and  $Z_3$  is the third degree orthogonal polynomial in  $z_b$ . From equation set (64) we see that

$$Z_1 = z_a,$$

$$Z_3 = z_b^3 - \left[ \frac{3(4)^2 - 7}{20} \right] z_b = z_b^3 - \left[ \frac{41}{20} \right] z_b.$$

Likewise,

$$Z_{00} = Z_0 Z_0 = (1)(1) = 1. \quad (83)$$

In equation (82) the terms  $\phi_{10} Z_{10}$  and  $\phi_{20} Z_{20}$  are the polynomial components of the true main effect of conditioning time. The terms  $\phi_{01} Z_{01}$ ,  $\phi_{02} Z_{02}$ , and  $\phi_{03} Z_{03}$  are the polynomial components of the true main effect of temperature. The terms  $\phi_{11} Z_{11}$ , . . . ,  $\phi_{23} Z_{23}$  are polynomial components of the true interaction effect between conditioning time and temperature.

Owing to the orthogonality of the  $Z_{ij}$ , the coefficients  $\phi_{ij}$  can be independently estimated from the values of the manganese recoveries. The estimated response equation will be of the form

$$\begin{aligned} y = & A^0 B^0 Z_{00} + AB^0 Z_{10} + A^0 B Z_{01} + A^2 B^0 Z_{20} + A^0 B^2 Z_{02} + A^0 B^3 Z_{03} \\ & + ABZ_{11} + AB^2 Z_{12} + AB^3 Z_{13} + A^2 B Z_{21} + A^2 B^2 Z_{22} + A^2 B^3 Z_{23}. \end{aligned} \quad (84)$$

The coefficients  $A^i B^j$  in equation (84) are coefficients of the polynomials  $Z_{ij}$  and are estimates of the coefficients  $\phi_{ij}$  in equation (82). In the coefficients  $A^i B^j$  any letter with a zero superscript may be conveniently omitted in the expression of the response function, and the letter  $I$  is herein used to represent  $A^0 B^0$  or any coefficient in which all letters have zero superscripts. Equation (84) then may be written

$$\begin{aligned} y = & IZ_{00} + AZ_{10} + BZ_{01} + A^2 Z_{20} + B^2 Z_{02} + B^3 Z_{03} + ABZ_{11} \\ & + AB^2 Z_{12} + AB^3 Z_{13} + A^2 B Z_{21} + A^2 B^2 Z_{22} + A^2 B^3 Z_{23}. \end{aligned} \quad (85)$$

As in the case of a single-factor experiment the  $A^i B^j$  are called coefficients of the polynomial components of the effects.

For the  $k$ 'th level of conditioning time and  $m$ 'th level of temperature the general relationship of equation (85) becomes

$$\begin{aligned} \bar{y}_{km} = & IZ_{00}(km) + AZ_{10}(km) + BZ_{01}(km) + A^2 Z_{20}(km) + B^2 Z_{02}(km) \\ & + B^3 Z_{03}(km) + ABZ_{11}(km) + AB^2 Z_{12}(km) + AB^3 Z_{13}(km) \\ & + A^2 B Z_{21}(km) + A^2 B^2 Z_{22}(km) + A^2 B^3 Z_{23}(km). \end{aligned} \quad (86)$$



When more than one factor is involved in an experiment, the subscript figures  $ij$  representing the degree of the  $Z_{ij}$  polynomials will be outside the parentheses, and the subscript figures  $km$  indicating the factor levels for the values of the  $Z_{ij}(km)$  will be inside the parentheses. There are  $km = (3)(4) = 12$  equations of the type shown in equation (86), and there are 12 unknowns  $I, A, B, \dots, A^2 B^3$ . The  $A^i B^j$  can, therefore, be resolved in terms of the  $Z_{ij}(km)$ , and the resulting general formula for the  $A^i B^j$  is

$$A^i B^j = \frac{\sum_{km} Z_{ij}(km) \bar{y}_{km}}{\sum_{km} Z_{ij}^2(km)} = \frac{\sum_{kmr} Z_{ij}(km) y_{kmr}}{Q \sum_{km} Z_{ij}^2(km)}. \quad (87)$$

From equations (87) and (83) we see that

$$I = A^0 B^0 = \frac{\sum_{km} Z_{00}(km) \bar{y}_{km}}{\sum_{km} Z_{00}^2(km)} = \frac{\sum_{km} \bar{y}_{km}}{12} = \bar{y}. \quad (88)$$

From equations (88), (84), and (83) we see that  $A^0 B^0 Z_{00} = I Z_{00} = I = \bar{y}$ , and equation (86) expresses each recovery as the sum of the experiment mean recovery and the polynomial components of the main effects and the interaction effects. When the  $A^i B^j$  have been determined, the relationships of equation sets (64) and (80) make it possible to convert equation (85) to the form,

$$\begin{aligned} y = & m_0 + m_a X_a + m_b X_b + m_{aa} X_a^2 + m_{bb} X_b^2 + m_{bbb} X_b^3 + m_{ab} X_a X_b \\ & + m_{abb} X_a X_b^2 + m_{abbb} X_a X_b^3 + m_{aab} X_a^2 X_b + m_{aabb} X_a^2 X_b^2 \\ & + m_{aabbb} X_a^2 X_b^3. \end{aligned} \quad (89)$$

The coefficients in equation (89) are estimates of the corresponding coefficients in the true response function of equation (79).

The values of the  $Z_{ij}(km)$  are the products of the corresponding  $Z_i(k)$  and  $Z_j(m)$ , and these are in turn related to the  $Z'_i(k)$  and the  $Z'_j(m)$  of table 1 by common factors  $W_i$  and  $W_j$ . It is, therefore, possible to express the  $A^i B^j$  of equation (87) in terms of  $\phi_{ij}$ ,  $W_{ij}$ , and  $Q_{ij}$ , so that

$$Z'_{ij} = W_{ij} Z_{ij}, \quad (90)$$

$$Z'_{ij}(km) = Z'_i(k) Z'_j(m), \quad (91)$$

$$Q_{ij} = \sum_{km} Z_{ij}^2(km) = \sum_k Z_i^2(k) \sum_m Z_j^2(m) = Q_i Q_j, \quad (92)$$

$$W_{ij} = W_i W_j, \quad (93)$$

$$\phi_{ij} = \sum_{kmr} Z'_{ij}(km) y_{kmr} = \sum_{km} Z'_i(k) \sum_r y_{kmr}. \quad (94)$$

From equations (87) and (90) to (94),

$$\begin{aligned} A^{ij} &= (\sum_{km} Z_{ij}(km) \bar{y}_{km}) / \sum_{km} Z_{ij}^2(km) \\ &= [\sum_{km} (Z'_{ij}(km) / W_{ij}) \bar{y}_{km}] / \sum_{km} (Z'_{ij}(km) / W_{ij})^2 \\ &= (W_{ij} / Q_{ij}) (\sum_{km} Z'_{ij}(km) \bar{y}_{km}) \end{aligned} \quad (95)$$

$$= (W_{ij} / Q_{ij}) (\sum_{kmr} Z'_{ij}(km) y_{kmr} / q) = (W_{ij} / q Q_{ij}) \phi_{ij}. \quad (96)$$

The calculation of the values for the  $Z'_{ij}(km)$ ,  $W_{ij}$ , and  $Q_{ij}$  can be conveniently made by a suitable array of the values followed by orderly multiplication. The necessary relationships for  $ij = 23$  are

$$Z'_{23}(km) = Z'_2(k) Z'_3(m),$$

$$W_{23} = W_2 W_3,$$

$$Q_{23} = Q_2 Q_3.$$

It should be noted that the values of  $W_2$  and  $Q_2$  are those associated with the values of  $Z'_2(k)$  and that the values of  $W_3$  and  $Q_3$  are those associated with the values of  $Z'_3(m)$ . A convenient symbolic arrangement of the calculation is

$Z'_{3(1)}$	$Z'_{3(2)}$	$Z'_{3(3)}$	$Z'_{3(4)}$	$W_3$	$Q_3$	(97a)
$Z'_{2(1)}$	$Z'_{2(2)}$	$Z'_{2(3)}$		$W_2$	$Q_2$	

$Z'_{2(1)} Z'_{3(1)}$	$Z'_{2(1)} Z'_{3(2)}$	$Z'_{2(1)} Z'_{3(3)}$	$Z'_{2(1)} Z'_{3(4)}$	$W_2 W_3$	$Q_2 Q_3$	(97b)
$Z'_{2(2)} Z'_{3(1)}$	$Z'_{2(2)} Z'_{3(2)}$	$Z'_{2(2)} Z'_{3(3)}$	$Z'_{2(2)} Z'_{3(4)}$			
$Z'_{2(3)} Z'_{3(1)}$	$Z'_{2(3)} Z'_{3(2)}$	$Z'_{2(3)} Z'_{3(3)}$	$Z'_{2(3)} Z'_{3(4)}$			

The products in the array (97b) are respectively equal to the corresponding quantities in the following array:

$Z'_{23(11)}$	$Z'_{23(12)}$	$Z'_{23(13)}$	$Z'_{23(14)}$	$W_{23}$	$Q_{23}$	(98)
$Z'_{23(21)}$	$Z'_{23(22)}$	$Z'_{23(23)}$	$Z'_{23(24)}$			
$Z'_{23(31)}$	$Z'_{23(32)}$	$Z'_{23(33)}$	$Z'_{23(34)}$			

The  $Z'_{23}(km)$  in the array (98) are the appropriate coefficients for the corresponding values of  $y_{km} = \sum_r y_{kmr}$  given in the array (77), which must be used to calculate the component coefficient  $A^2 B^3$  according to equations (94) and (96).

From table 1 the actual data for the calculation of the  $Z'_{23}(\text{km})$ ,  $W_{23}$ , and  $Q_{23}$  were obtained and the calculation made as shown in the array 99a-b:

<u>Factor level</u>							
n	$Z'$	1	2	3	4	Q	W
4	$Z'_{3(m)}$	-1	+3	-3	+1	20	10/3
3	$Z'_{2(k)}$	+1	-2	+1		6	3
12	$Z'_{23}(\text{km})$	-1	+3	-3	+1	120	10
		+2	-6	+6	-2		
		-1	+3	-3	+1		

(99a)

(99b)

According to equation (94),

$$\phi_{23} = \sum_{km} Z'_{23}(\text{km}) \sum_r y_{kmr} = \sum_{km} Z'_{23}(\text{km}) y_{km}. \quad (100)$$

When the  $Z'_{23}(\text{km})$  of the array (99b) are multiplied by the corresponding values of  $y_{km}$  in the array (77) and the 12 products are summed, the result is

$$\begin{aligned} \phi_{23} = & (-1)(154) + (3)(156) + (-3)(158) + (1)(160) \\ & + (2)(158) + (-6)(162) + (6)(164) + (-2)(166) \\ & + (-1)(160) + (3)(164) + (-3)(168) + (1)(170) = -6. \end{aligned}$$

From equation (96) we obtain

$$A^2 B^3 = (W_{23}/Q_{23}) \phi_{23} = [10/2(120)](-6) = -1/4. \quad (101)$$

The values of  $Z'_{ij}(\text{km})$ ,  $W_{ij}$ , and  $Q_{ij}$  were calculated for all the terms of equation (86) and are listed in table 2.

For the purpose of later developments it is noted here that

$$\sum_k Z'_{ij}(\text{km}) = \sum_k Z'_{i(k)} Z'_{j(m)} = Z'_{j(m)} \sum_k Z'_{i(k)} = 0. \quad (102)$$

The relationship of equation (102) holds true for all  $Z'_{ij}(\text{km})$  except  $Z'_{00}(\text{km})$ , providing that the summation is performed over levels of a factor for which  $i \neq 0$  in equation (102). This characteristic may be observed for the  $Z'_{ij}(\text{km})$  of table 2. The values of the component coefficients,  $A^i B^j$ , for all terms of equation (86) were calculated and listed in table 3.



TABLE 2. - Values of the orthogonal polynomials for a three-level  
by four-level experiment with two factors

$Z'$	Factor level, m				Q	W
	1	2	3	4		
$Z'_{23}(\text{km})$	-1	+3	-3	+1	120	10
	+2	-6	+6	-2		
	-1	+3	-3	+1		
$Z'_{22}(\text{km})$	+1	-1	-1	+1	24	3
	-2	+2	+2	-2		
	+1	-1	-1	+1		
$Z'_{21}(\text{km})$	-3	-1	+1	+3	120	6
	+6	+2	-2	-6		
	-3	-1	+1	+3		
$Z'_{13}(\text{km})$	+1	-3	+3	-1	40	10/3
	0	0	0	0		
	-1	+3	-3	+1		
$Z'_{12}(\text{km})$	-1	+1	+1	-1	8	1
	0	0	0	0		
	+1	-1	-1	+1		
$Z'_{11}(\text{km})$	+3	+1	-1	-3	40	2
	0	0	0	0		
	-3	-1	+1	+3		
$Z'_{03}(\text{km})$	-1	+3	-3	+1	60	10/3
	-1	+3	-3	+1		
	-1	+3	-3	+1		
$Z'_{02}(\text{km})$	+1	-1	-1	+1	12	1
	+1	-1	-1	+1		
	+1	-1	-1	+1		
$Z'_{01}(\text{km})$	-3	-1	+1	+3	60	2
	-3	-1	+1	+3		
	-3	-1	+1	+3		
$Z'_{20}(\text{km})$	+1	+1	+1	+1	24	3
	-2	-2	-2	-2		
	+1	+1	+1	+1		
$Z'_{10}(\text{km})$	-1	-1	-1	-1	8	1
	0	0	0	0		
	+1	+1	+1	+1		
$Z'_{00}(\text{km})$	+1	+1	+1	+1	12	1
	+1	+1	+1	+1		
	+1	+1	+1	+1		

TABLE 3. - Values for the coefficients of the polynomial components of effects for a two-factor, three-level by four-level, hypothetical manganese flotation experiment

ij	$\phi_{ij}$	$\phi_{ij} W_{ij} / qQ_{ij}$	Component coefficients, $A^i B^j$
23	-6	$(-6)(10)/2(120)$	-1/4
22	2	$(2)(3)/2(24)$	1/8
21	2	$(2)(6)/2(120)$	1/20
13	-2	$(-2)(10/3)/2(40)$	-1/12
12	-2	$(-2)(1)/2(8)$	-1/8
11	14	$(14)(2)/2(40)$	7/20
03	0	0	0
02	-4	$(-4)(1)/2(12)$	-1/6
01	80	$(80)(2)/2(60)$	4/3
20	-10	$(-10)(3)/2(24)$	-5/8
10	34	$(34)(1)/2(8)$	17/8
00	1940	$(1940)(1)/2(12)$	80-5/6

The  $ij$ 'th component of the effects in equation (86) can be determined for any of the  $\bar{y}_{km}$  by multiplying the corresponding value of  $Z_{ij(km)}$  by the value of the  $ij$ 'th component coefficient from table 3. The values of  $Z_{ij(km)}$  are determined from table 2 by the relationship  $Z_{ij(km)} = Z'_{ij(km)} / W$ . For example,  $A^2 B^3 = -1/4$ ,  $Z_{23(11)} = -1/10$ , and the quadratic A by cubic B component of the interaction effect between conditioning time and temperature for the average manganese recovery  $y_{11}$  is

$$A^2 B^3 Z_{23(11)} = (-1/4)(-1/10) = 1/40.$$

A numerical check on the calculations for the results shown in table 3 can be made by calculating and summing all of the polynomial components for any mean recovery  $\bar{y}_{km}$  and by adding the sum to the experiment mean recovery,  $\bar{y}$ . The result should be equal to the mean recovery,  $\bar{y}_{km}$ . For example, we obtain from equation (86),

$$\begin{aligned} \bar{y}_{11} = \bar{y} &+ AZ_{10(11)} + A^2 Z_{20(11)} + BZ_{01(11)} + B^2 Z_{02(11)} + B^3 Z_{03(11)} \\ &+ ABZ_{11(11)} + AB^2 Z_{12(11)} + AB^3 Z_{13(11)} + A^2 BZ_{21(11)} \\ &+ A^2 B^2 Z_{22(11)} + A^2 B^3 Z_{23(11)}. \end{aligned} \quad (103)$$

When the values of  $A^i B^j$  and  $Z_{ij(11)}$  are substituted in equation (103) the result is

$$\begin{aligned} \bar{y}_{11} &= 80-5/6 + (17/8)(-1) + (4/3)(-3/2) + (-5/8)(1/3) + (-1/6)(1) \\ &+ (0)(-3/10) + (7/20)(3/2) + (-1/8)(-1) + (-1/12)(3/10) \\ &+ (1/20)(-3/6) + (1/8)(1/3) + (-1/4)(-1/10) \\ &= 77. \end{aligned}$$

The value of  $\bar{y}_{11} = 77$  percent manganese recovery checks with the value originally given in the array (78).

### Transformation of Many-Factor Response Functions

The orthogonal transformation of the response function to calculate the polynomial main effects and interaction effects of an experiment with any number of factors having equally spaced levels is a simple extension of the calculations for one and two factors. The  $Z'$ ,  $W$ , and  $Q$  for any component effect is the product of the individual  $Z'$ ,  $W$ , and  $Q$  associated with the power of each factor involved in the aforesaid component effect. Consider the calculation of the interaction coefficient  $AC^2$  for an experiment with four factors with levels and replication as follows:

<u>Factor</u>	<u>Factor Levels</u>	
$X_a$	$k = 1, \dots, s$	
$X_b$	$m = 1, \dots, t$	
$X_c$	$n = 1, \dots, u$	(104)
$X_d$	$p = 1, \dots, v$	
Replication	$r = 1, \dots, q$	

The coefficient  $AC^2$  is calculated as follows:

$$AC^2 = A^1 B^0 C^2 D^0 = \phi_{1020} W_{1020} / q Q_{1020}, \quad (105)$$

$$\phi_{1020} = \sum_{kmnp} Z'_{1020}(kmnp) \sum_r y_{kmnp r}, \quad (106)$$

$$Z'_{1020}(kmnp) = Z'_1(k) Z'_0(m) Z'_2(n) Z'_0(p) = Z'_1(k) Z'_2(n), \quad (107)$$

$$W_{1020} = W_1(k) W_0(m) W_2(n) W_0(p) = W_1(k) W_2(n), \quad (108)$$

$$\begin{aligned} Q_{1020} &= Q_1(k) Q_0(m) Q_2(n) Q_0(p) = Q_1(k) t Q_2(n)^v \\ &= tv Q_1(k) Q_2(n). \end{aligned} \quad (109)$$

It should be noted that in equation (105) the interaction coefficient  $AC^2$  was first expressed as a product involving all factors by the equivalent expression  $A^1 B^0 C^2 D^0$ . The subscripts on the quantities  $\phi_{1020}$ ,  $Z'_{1020}$ ,  $W_{1020}$ , and  $Q_{1020}$  are the same as the superscripts on the letters in the expression  $A^1 B^0 C^2 D^0$ , and are in the same order. The successive numbers in the subscript 1020 properly identify the one-factor orthogonal polynomials that must be multiplied together to obtain the orthogonal polynomial which the coefficient  $AC^2$  modifies. The letters  $k$ ,  $m$ ,  $n$ , and  $p$  in the subscripts of equations (107), (108), and (109) serve to identify the values of  $Z'$ ,  $W$ , and  $Q$  which must be selected from table 1 for the respective values of  $s$ ,  $t$ ,  $u$ , and  $v$ , the total number of levels per factor. This general procedure will work for the coefficient of any polynomial effect, whatever the number of factors may be.



### The Algebraic Expression of Design Relationships

The theoretical relationship between an observation in an experiment, the effects of the factors, and the errors involved in an experiment may be conveniently assumed or postulated in the form of a statistical model to facilitate proper design and subsequent analysis of experimental data. A statistical model is an algebraic equation that symbolically indicates the theoretical division of an observation into suitable components, including the experiment mean and the experimental error. For quantitative factors the other components may be either effects or polynomial components of effects. When polynomial components are involved, we also have a response equation if all of the factors are quantitative. For qualitative factors the components other than the mean and the experimental error are only the effects. The use of models provides a convenient and systematic method of evaluating the importance of effects for both quantitative and qualitative factors without reference to polynomial components.

A simple one-factor model may be developed on the basis of previous discussion on orthogonal transformations. Consider the general case, previously discussed, of the one-factor experiment with the true response function shown in equation (56); namely,

$$Y = M_0 + M_a X_a + M_{aa} X_a^2 + \dots + M_{aa\dots a} X_a^{n-1}.$$

The orthogonal transformation of equation (56) was given in equation (61) as follows:

$$Y = \phi_0 Z_0 + \phi_1 Z_1 + \phi_2 Z_2 + \dots + \phi_{n-1} Z_{n-1}.$$

For the purpose of developing the theory of models let  $\phi_2 Z_2$  of equation (61) be called  $*A^2$  and in general let

$$*A^i = \phi_i Z_i. \quad (110)$$

The quantities  $*A^i$ ,  $i = 1, \dots, (n-1)$ , are, therefore, defined to be the components of the true effect,  $*A$ , of the factor  $X_a$ ; that is,

$$*A = *A + *A^2 + \dots + *A^{n-1}. \quad (111)$$

For the  $k$ 'th level of factor  $X_a$ ,

$$*A_k = *A_k + *A_k^2 + \dots + *A_k^{n-1}. \quad (112)$$

For the  $k$ 'th level of factor  $X_a$  the estimated response function for equation (61) was shown in equation (66) as

$$\bar{y}_k = A^0 Z_{0k} + A Z_{1k} + A^2 Z_{2k} + \dots + A^{n-1} Z_{(n-1)k}.$$

The term  $A^0 Z_{0k}$  in equation (66) is an estimate of  $\phi_0 Z_{0k} = *A_k^0$ , and since  $A^0 Z_{0k} = \bar{y}$ ,  $\bar{y}$  is an estimate of  $*A_k^0$ . If  $\mu$  is the true mean response of the

experiment, then  $\bar{y}$  is an estimate of  $\mu$  and  $*A_k^0$  is the same as  $\mu$ . If  $A_{ik}^i Z_{ik} = A_k^i$ , equation (66) then may be written

$$\bar{y}_k = \bar{y} + A_k + A_k^2 + \dots + A_k^{n-1}, \quad (113)$$

$$\bar{y}_k = \bar{y} + \underline{A}_k. \quad (114)$$

$$A_k^i = \text{estimate of } *A_k^i,$$

$$\underline{A}_k = \text{estimate of } *A_k.$$

In equation (114)  $\bar{y}_k$  is an estimate of the true mean,  $\mu_k$ , at the  $k$ 'th level of factor  $X_a$ . Equation (114) is an estimate of the equation

$$\mu_k = \mu + *A_k. \quad (115)$$

Equation (115) is equivalent to the equation

$$y_{kr} = \mu + *A_k + *e_{r(k)}. \quad (116)$$

$$*e_{r(k)} = y_{kr} - \mu_k.$$

Equation (116) is the statistical model for a one-factor experiment. The quantity  $*e_{r(k)}$  is the true error in the observation  $y_{kr}$ . The replicate number represented by the letter  $r$  is placed last in the subscript of the observation,  $y_{kr}$ , but is placed first in the subscript of the error term,  $*e_{r(k)}$ , whereas the factor level is placed in parentheses in the subscript of the error term. This order in the subscript of experimental error is not always used in the current literature but is followed in this report.

Equation (116) was developed for the general case of an experiment in which the factor was quantitative and the effect of the factor could have polynomial components. On the basis of equation (112) the model could be expanded as follows:

$$y_{kr} = \mu + *A_k + *A_k^2 + \dots + *A_k^{n-1} + *e_{r(k)}. \quad (117)$$

Although equation (116) was developed for a quantitative factor, the same equation may be used for a model of an experiment with one qualitative factor. However, there would not be any polynomial components, and the model could not be expanded to the form of equation (117). In the case of both quantitative and qualitative factors, equation (116) is a proper expression of the model, and the true main effect  $*A_k$  is the difference between the true experiment mean and the true mean at the  $k$ 'th level, that is, from equation (115),

$$*A_k = \mu_k - \mu. \quad (118)$$

The model for a two-factor experiment may be developed on the basis of previous discussion on orthogonal transformation. Consider the two-factor manganese experiment, previously discussed, in which conditioning time was

factor  $X_a$  with levels  $k = 1, 2, 3$ ; temperature was factor  $X_b$  with levels  $m = 1, 2, 3, 4$ ; and replication was  $r = 1, 2$ . The true response function was given in equation (79) as follows:

$$Y = M_0 + M_a X_a + M_b X_b + M_{aa} X_a^2 + M_{bb} X_b^2 + M_{bbb} X_b^3 + M_{ab} X_a X_b \\ + M_{abb} X_a X_b^2 + M_{abbb} X_a X_b^3 + M_{aab} X_a^2 X_b + M_{aabb} X_a^2 X_b^2 \\ + M_{aabbb} X_a^2 X_b^3.$$

The orthogonal transformation of equation (79) was shown in equation (82) as

$$Y = \phi_{00} Z_{00} + \phi_{10} Z_{10} + \phi_{01} Z_{01} + \phi_{20} Z_{20} + \phi_{02} Z_{02} + \phi_{03} Z_{03} \\ + \phi_{11} Z_{11} + \phi_{12} Z_{12} + \phi_{13} Z_{13} + \phi_{21} Z_{21} + \phi_{22} Z_{22} + \phi_{23} Z_{23}.$$

The term  $\phi_{23} Z_{23}$  from equation (82) is called  $*A^2 B^3$ , and in general,

$$*A^i B^j = \phi_{ij} Z_{ij}. \quad (119)$$

According to equation (119), the quantities  $*A^i = *A^i B^0$ ,  $i = 1, 2$  are defined as the components of the true main effect of conditioning time, the quantities  $*B^j = *A^0 B^j$ ,  $j = 1, 2, 3$  are defined as the components of the true main effect of temperature, and the quantities  $*A^i B^j$ ,  $i, j \neq 0$  are defined as the components of the true interaction effect of conditioning time and temperature.

Let the true main effect of conditioning time, the true main effect of temperature, and the true interaction effect of the two factors be  $*A$ ,  $*B$ , and  $*AB$ , respectively. For the  $k$ 'th level of conditioning time and the  $m$ 'th level of temperature the following relationships then hold:

$$*A_k = *A_k + *A_k^2, \\ *B_m = *B_m + *B_m^2 + *B_m^3, \\ *AB_{km} = (*AB)_{km} + (*AB^2)_{km} + (*AB^3)_{km} + (*A^2 B)_{km}, \\ + (*A^2 B^2)_{km} + (*A^2 B^3)_{km}. \quad (120)$$

For the  $k$ 'th level of conditioning time and the  $m$ 'th level of temperature, the estimated response function for equation (82) was given in the form shown in equation (86); namely,

$$\bar{y}_{km} = IZ_{00}(km) + AZ_{10}(km) + BZ_{01}(km) + A^2 Z_{20}(km) + B^2 Z_{02}(km) \\ + B^3 Z_{03}(km) + ABZ_{11}(km) + AB^2 Z_{12}(km) + AB^3 Z_{13}(km) \\ + A^2 BZ_{21}(km) + A^2 B^2 Z_{22}(km) + A^2 B^3 Z_{23}(km).$$



Let the nomenclature for the terms in equation (86) be changed as follows:

$$\begin{aligned} A^i Z_{io(km)} &= A_k^i, \\ B^j Z_{oj(km)} &= B_m^j, \\ A^i B^j Z_{ij(km)} &= (A^i B^j)_{km}. \end{aligned} \quad (121)$$

By means of the equalities in equation set (121) and the fact that  $I Z_{oo(km)} = \bar{y}$ , equation (86) may be written

$$\begin{aligned} \bar{y}_{km} &= \bar{y} + A_k + A_k^2 + B_m + B_m^2 + B_m^3 + (AB)_{km} + (AB^2)_{km} \\ &\quad + (AB^3)_{km} + (A^2 B)_{km} + (A^2 B^2)_{km} + (A^2 B^3)_{km}, \end{aligned} \quad (122)$$

$$\bar{y}_{km} = \bar{y} + \underline{A}_k + \underline{B}_m + \underline{AB}_{km}. \quad (123)$$

$$A_k^i = \text{estimate of } *A_k^i,$$

$$B_m^j = \text{estimate of } *B_m^j,$$

$$(A^i B^j)_{km} = \text{estimate of } (*A^i B^j)_{km},$$

$$\underline{A}_k = \text{estimate of } *A_k,$$

$$\underline{B}_m = \text{estimate of } *B_m,$$

$$\underline{AB}_{km} = \text{estimate of } *AB_{km}.$$

In equation (123)  $\bar{y}_{km}$  is an estimate of the true mean,  $\mu_{km}$ , at the levels  $k$  and  $m$ . Equation (123) is an estimate of the equation,

$$\mu_{km} = \mu + *A_k + *B_m + *AB_{km}, \quad (124)$$

$$*A_k = \mu_k - \mu,$$

$$*B_m = \mu_m - \mu,$$

$$*AB_{km} = \mu_{km} - (\mu + *A_k + *B_m) = \mu_{km} - \mu_k - \mu_m + \mu.$$

Equation (124) is equivalent to the equation,

$$y_{kmr} = \mu + *A_k + *B_m + *AB_{km} + *e_{r(km)}, \quad (125)$$

$$*e_{r(km)} = y_{kmr} - \mu_{km}.$$

Equation (125) is the statistical model for a two-factor experiment with factors  $X_a$  and  $X_b$ . The quantity  $*e_{r(km)}$  is the true error in the observation  $y_{kmr}$ .

Because conditioning time and temperature were quantitative factors with three and four levels, respectively, the model could be expanded on the basis of equation set (120) as follows:

$$y_{kmr} = \mu + *A_k + *A_k^2 + *B_m + *B_m^2 + *B_m^3 + (*AB)_{km} \\ + (*AB^2)_{km} + (*AB^3)_{km} + (*A^2B)_{km} + (*A^2B^2)_{km} \\ + (*A^2B^3)_{km} + *e_{r(km)}. \quad (126)$$

However, if one or both of the factors had been qualitative, equation (126) would not be, but equation (125) would be, a proper expression for the model.

If one factor was quantitative and one factor was qualitative, the model of equation (125) could be expanded for components of the quantitative factor. It is possible for such components to vary from level to level of the qualitative factor and to produce interactions between the components and the main effect of the qualitative factor. For example, suppose that factor  $X_a$  was quantitative and factor  $X_b$  was qualitative. In conformity with previous notation the true interaction of the linear component of  $*A$  with  $*B$  for the levels  $k$  and  $m$  would be designated by  $(*AB)_{km}$ . The true interaction between the quadratic component of  $*A$  and the main effect  $*B$  for the levels  $k$  and  $m$  would be  $(*A^2B)_{km}$ . The relationship of these quantities is

$$*AB_{km} = (*AB)_{km} + (*A^2B)_{km}. \quad (127)$$

With the notation of equation (127) the model of equation (125) could be expanded to

$$y_{kmr} = \mu + *A_k + *A_k^2 + *B_m + (*AB)_{km} + (*A^2B)_{km} + *e_{r(km)}. \quad (128)$$

Since the notation of the effects and their components for interactions can be rather cumbersome with increased number of factors, the letter  $*I$  with a subscript indicating the factor levels involved has been adopted for the general expression of some models in this report. This notation can be used for all of the unexpanded models such as the two-factor model of equation (125); that is,

$$y_{kmr} = \mu + *A_k + *B_m + *I_{km} + *e_{r(km)}. \quad (129)$$

When all of the factors are quantitative as in the case of the two-factor model of equation (126), the general expanded model can be written

$$y_{kmr} = \mu + *A_k + *A_k^2 + *B_m + *B_m^2 + *B_m^3 + *I_{km}^{11} + *I_{km}^{12} \\ + *I_{km}^{13} + *I_{km}^{21} + *I_{km}^{22} + *I_{km}^{23} + *e_{r(km)}. \quad (130)$$

The meaning of the notations in equation (130) is illustrated by the meaning of  $I_{km}^{21}$ , namely,  $I_{km}^{21}$  is the quadratic A and the linear B interaction at the  $k$ 'th level of factor  $X_a$  and the  $m$ 'th level of factor  $X_b$ . When some, but not

all, of the factors are qualitative as in the case of the model in equation (128), the expanded model can be written

$$y_{kmr} = \mu + *A_k + *A_k^2 + *B_m + *I_{km}^1 + I_{km}^2 + *e_{r(km)}. \quad (131)$$

In equation (131) the letter m in the superscript of  $*I_{km}^2$  indicates that the main effect  $*B_m$  is involved in the interaction rather than a component of  $*B_m$ .

For most purposes of experiment design it is adequate to express a statistical model in the shorter form similar to equations (116), (125), and (129). An appreciation of the possible importance of some of the polynomial components is sufficient to insure consideration of an adequate number of factor levels in a design to investigate such components.

An important feature of a model such as (130) for which the factors are quantitative is that the summation of any polynomial component over all design levels of any factor involved in the component is zero. This feature is illustrated in the case of the estimated effect  $I_{km}^{23}$  for the model; that is,

$$I_{km}^{23} = (A^2 B^3)_{km} = A^2 B^3 Z_{23}(km),$$

$$\sum_m I_{km}^{23} = \sum_m A^2 B^3 Z_{23}(km) = A^2 B^3 \sum_m Z_{23}(km) = (A^2 B^3 / W_{23}) \sum_m Z'_{23}(km) = 0.$$

This result is confirmed by equation (102). In general,

$$\sum_m I_{km}^{ij} = \sum_k I_{km}^{ij} = 0. \quad (132)$$

As a consequence of these relationships the summation of any effect for such a model over all design levels of a factor involved in the effect is zero. This is illustrated for the unexpanded form of the model as shown in (129); that is,

$$I_{km} = \sum_{ij} I_{km}^{ij},$$

$$\sum_k I_{km} = \sum_m I_{km} = \sum_m \sum_{ij} I_{km}^{ij} = \sum_{ij} \sum_m I_{km}^{ij} = 0. \quad (133)$$

Results similar to those of (133) are easily demonstrated for main effects. Although the results were demonstrated for quantitative factors, they also apply to the effects of qualitative factors.

#### Crossed Classification

Models generally are classified for convenient reference as being either crossed or nested. Some models have both of these characteristics. Equation (129) is an example of a model with a two-way crossed classification. Crossed classification exists when (1) each factor level in an experiment occurs with one or more levels from each of the other factors and (2) every observation of the response for each test having a specific factor level contains an effect both constant and peculiar to that factor level.



Examples of crossed classified models for three- and four-factor experiments are shown in equations (134) and (135):

$$y_{kmnr} = \mu + *A_k + *B_m + *C_n + *I_{km} + *I_{kn} + *I_{mn} + *I_{kmn} + *e_r(kmn), \quad (134)$$

$$y_{kmnpr} = \mu + *A_k + *B_m + *C_n + *D_p + *I_{km} + *I_{kn} + *I_{kp} + *I_{mn} + *I_{mp} + *I_{np} + *I_{kmn} + *I_{kmp} + *I_{knp} + *I_{mnp} + *I_{kmnp} + *e_r(kmnp). \quad (135)$$

In any model it is possible that any one or all of the interaction effects could be postulated to be absent on the basis of prior knowledge. All of the common statistical models may be considered either as examples of crossed classification or as special cases of crossed classification either with or without the occurrence of nested classification. An example of such a special case is the model of equation (116) which may be described as having a one-way crossed classification because only one factor is involved.

#### Nested Classification

The term nested classification describes a model for a design or a fraction of a design in which there is a successive replication of a factor level or levels associated with each replication of some preceding factor level or levels. For example, suppose that three batches of ore were sampled from a carload of ore, three samples were taken from each batch, and two chemical analyses were made on each sample. The three batches of ore are replicates, the nine samples are replicates of three within batches, and the eighteen analyses are replicates of two within samples. This is illustrated in figure 7.

The replicate batches, samples, and analyses of figure 7 may be numbered in any possible order; for example, the batches can be ordered xyz as shown in figure 7 or they could be ordered yzx, zxy, yxz, xzy, or zyx. Only the sam-

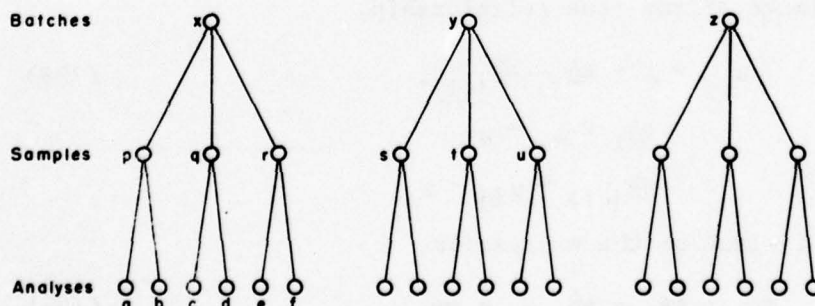


FIGURE 7. - A Design With a Nested Classification.

ples within a particular batch can be ordered; that is, the samples from batch y could be ordered stu, tus, ust, sut, uts, or tsu. Likewise only the analyses on a particular sample can be ordered; for example, the analyses for sample q could be ordered cd or dc.

In general, a peculiarity of nesting is that there is no correlation between the occurrence of a particular numbered replicate of a factor  $X_b$  nested within a replicate of a factor  $X_a$  and the occurrence of a replicate of  $X_b$  with the same number within another replicate of  $X_a$ , irrespective of the order in which the replicates may be numbered. Furthermore, the replicates of  $X_b$  having the same number from replicate to replicate of  $X_a$  do not have a constant and common effect. Under such conditions interactions do not exist between the factors  $X_a$  and  $X_b$ .

Assume that the response for the design of figure 7 is percent lead in the ore. Let batches be factor  $X_a$  with replicates  $i = 1, 2$ , and 3. Let samples be factor  $X_b$  with replicates  $j = 1, 2$ , and 3. The main purpose of the sampling experiment is to examine the errors due to sampling, and therefore, only batches and samples are formally classified as factors. The duplication of analyses is for determining error due to chemical analysis and would not be necessary if the chemist already has a good estimate of the error due to analytical procedures. Let the replicate analyses be  $k = 1, 2$ . The percent lead for the  $k$ 'th replicate analysis of the  $j$ 'th sample from the  $i$ 'th batch is represented by  $y_{ijk}$ . The mean value of both replicate lead analyses of the  $j$ 'th sample from the  $i$ 'th batch is represented by  $\bar{y}_{ij}$ . The mean value of all the lead analyses in the design is represented by  $\bar{y}$ . The difference between these two mean analyses is equal to the combined effect upon the lead analysis of the procedures used in selecting the batches and the samples. This fact is expressed by the equation

$$\bar{y}_{ij} - \bar{y} = \underline{A}_i + \underline{B}_{j(i)}. \quad (136)$$

In equation (136) the subscript of  $\underline{B}_{j(i)}$  indicates that the  $j$ 'th replicate sample is nested within the  $i$ 'th replicate batch.

Rearrangement of equation (136) shows that the mean lead analysis  $\bar{y}_{ij}$  is equal to the experiment mean analysis plus the effects due to selecting the batches and the samples; that is,

$$\bar{y}_{ij} = \bar{y} + \underline{A}_i + \underline{B}_{j(i)}. \quad (137)$$

Equation (137) is an estimate of the true relationship,

$$\mu_{ij} = \mu + *A_i + *B_{j(i)}. \quad (138)$$

$$*A_i = \mu_i - \mu$$

$$*B_{j(i)} = \mu_{ij} - \mu_i$$

Equation (138) is the equivalent of the expression,

$$y_{ijk} = \mu + *A_i + *B_{j(i)} + *e_{k(ij)}. \quad (139)$$

$$*e_{k(ij)} = y_{ijk} - \mu_{ij}$$

Equation (139) is a two-factor statistical model with a nested classification. The term  $\mu_{j(i)}$  is read "the true effect B underline sub j within i" and the error term  $\epsilon_{k(ij)}$  is read "e sub k within ij." In each case of nested replicates, the factor replicates within which another replicate is nested are placed within parentheses which occur last in the subscript. The order of the factor replicates within the parentheses is the same as their order in the subscript of the observation. An important point concerning the model shown in equation (139) is that the model is true for any actual observation  $y_{ijk}$ , irrespective of how many other observations may be obtained. For example, the model is true for the case of an experiment with one batch, one sample from that batch, and only one analysis for the sample. This illustrates a characteristic of the relationship between models and designs; namely, it is possible for many designs to have the same model.

The extension of these ideas to cases in which greater numbers of factors are nested is easily made. With reference to nested classification the term rank is used to indicate the position of a nested factor. The model of equation (139) is called a two-rank nested model. Batches are the first rank, and samples are the second rank. Only primary factors under investigation are referred to in the classification of nested models. The term rank originated from the idea of a hierarchical relationship between the successive factors of a nested classification. In the literature the terms hierarchic and nested are used synonymously.

The variety of ways in which nesting can occur within a crossed classification is considerable, and the proper expression of a model with these two characteristics is an aid both to proper design and to the ease of subsequent analysis of the experimental data. An illustration of a problem involving a model with both a crossed and nested classification is given in the section on nested designs.

### Factorial Designs

When experiments are designed statistically, it is possible to estimate important effects, to obtain quantitative measures of the confidence to be placed in the estimates, to compare the relative importance of the various effects, and to calculate empirical or theoretical mathematical relationships between the factors and the response. When experiments are not statistically designed, attempts to evaluate relatively large amounts of data by statistical methods are frequently disappointing. Sometimes the information contained in the data may be sketchy and, therefore, only a few rough comparisons can be made, or perhaps some important effects actually are confused so that separate estimates of these effects cannot be obtained.

If only the main effects of several factors are important and no significant interactions exist, then the classical method can be used, in which the effect of one factor is estimated by a series of tests in which that one factor is varied and all others are held constant. This method is continued until all factors have been investigated separately. If there were a possibility of interaction effects between the factors, however, the classical



approach would not detect nor yield estimates of such effects. Furthermore, when only main effects are important, certain statistical designs may yield the desired information with fewer tests than are required by a classical approach and will provide additional information concerning the statistical reliability of results obtained.

The factorial design, one of the more important statistical designs, is one in which several factors may be studied at a specified number of levels with all possible combinations of the factor levels included in the design. Such a design may be used to investigate the effects of both qualitative and quantitative factors. The main and interaction effects which involve only quantitative factors may be analyzed for linear, quadratic, cubic, and higher order components, depending upon the number of levels chosen for these factors. With factorial designs it is possible to obtain independent estimates of main effects and all possible interaction effects of the factors being studied. Interaction effects are common between chemical and physical factors. For example, the time to reach maximum metal reduction may decrease as roasting temperature is increased, or the best leaching temperature at one pH value may not be the best temperature at another pH value. Experience with specific systems of physicochemical factors, however, may have demonstrated that certain factors do not interact, and such experience should be used in planning the research program. However, in the absence of previous evidence, it is unwise to assume that factors do not interact.

A factorial design for the manganese flotation experiment in which three levels, 3, 4, and 5 minutes, are selected for conditioning time and four levels, 30°, 40°, 50°, and 60° C., are selected for temperature includes the 12 possible combinations of these factor levels. From the results of an experiment based on this design it is possible to estimate the linear and quadratic components of the main effect of conditioning time; linear, quadratic, and cubic components of the main effect of temperature; and six components of the interaction effect between the two factors.

If some of the interaction effects are not important, it may be possible to use a fractional factorial design in which only those tests which are sufficient for estimating the important effects are selected from the corresponding full factorial design. Fractional factorial designs have the advantage of reducing the number of tests to be made and yet have some of the properties of full factorial designs. The principles underlying fractional factorial designs must be understood before attempting to use them, however, or else important effects may be confused so that they cannot be estimated separately.

The following notation is used to represent the individual tests in a design in order to facilitate explanation of the properties of factorial designs. When a single quantitative factor  $X_a$  is to be tested at several levels, the test made at the lowest level is represented by  $a_0$ , and the tests made at successively higher levels are represented by  $a_1$ ,  $a_2$ ,  $a_3$ , and so forth. This system of numbering for the subscripts simplifies the later application of principles from mathematical group theory to determine the tests which are to be included in a fractional factorial design. It must be remembered that the response  $y_1$  corresponds to test  $a_0$ ,  $y_2$  to  $a_1$ , and so on. In general, the

subscript for the test symbol is one less than that for the corresponding response. The levels of a qualitative factor may be arranged in any convenient order so as to use this notation when referring to the tests made.

The notation is extended to experiments involving more than one factor. In the manganese flotation experiment, let  $X_a$  represent time and  $X_b$  represent temperature. The letters a and b with appropriate subscripts identify the levels of factors  $X_a$  and  $X_b$ , respectively, in the test symbols for this experiment. The test made at the second level of conditioning time, 4 minutes, and third level of temperature, 50° C., is represented by the symbol  $a_1 b_2$ . An additional advantage of simplicity in notation is gained if the letter corresponding to a particular factor is omitted whenever that factor is at its lowest level. Thus, the test made for 5 minutes at 30° C. is represented by  $a_2$ , the test made for 3 minutes at 40° C. is represented by  $b_1$ , etc. The test made at the lowest level of all factors is represented by (1). This last symbol is chosen for its correspondence with the concept of an identity in group theory and further simplifies the procedures for determining the tests to be included in a fractional factorial design. The 12 tests in the factorial design for the manganese flotation experiment are shown in table 4 together with the appropriate test symbols.

TABLE 4. - Tests in a factorial experiment to investigate recovery of manganese by flotation in which three levels of conditioning time and four levels of temperature are studied

Test symbol	Conditioning time, minutes	Temperature, ° C.
(1)	3	30
$a_1$	4	30
$a_2$	5	30
$b_1$	3	40
$a_1 b_1$	4	40
$a_2 b_1$	5	40
$b_2$	3	50
$a_1 b_2$	4	50
$a_2 b_2$	5	50
$b_3$	3	60
$a_1 b_3$	4	60
$a_2 b_3$	5	60

The independence of estimates of the various effects measured in a factorial experiment depends upon the number of times each test in the design is made. Suppose that each of the tests in the full factorial design for the manganese flotation experiment were made twice to obtain an estimate of experimental error as well as estimates of the various factor effects. An average manganese recovery for 3 minutes' conditioning time then can be calculated



from the results of eight tests, two tests made at each of the four levels of temperature. Similar average manganese recoveries can be calculated for 4 and 5 minutes' conditioning time. Since each average is obtained from the same number of tests at each of the levels of temperature, comparisons which are independent of temperature can be made between these average recoveries for the three levels of conditioning time. Comparisons which are independent of conditioning time also can be made between average recoveries for the four levels of temperature. Independent estimates of the main effects of time and temperature are obtained by means of these comparisons. The data also will yield an estimate of the interaction effect between time and temperature which is independent of both main effects. A design that will give independent estimates of all important effects is said to be orthogonal.

If one of the tests in a factorial design were not made, the experiment would not be orthogonal. Suppose the test  $a_1 b_2$  for 4 minutes at 50° C. were omitted, but the other 11 tests in the design were each made once, then the average manganese recovery for 4 minutes is obtained over only three levels of temperature, whereas the average recoveries for 3 and 5 minutes are obtained over four levels of temperature. Also, the average recovery at 50° C. is obtained only over two levels of conditioning time, whereas the average recoveries at 30°, 40°, and 60° C. are obtained over three levels of time. Comparisons between averages for different levels of time will not be independent of temperature, nor will comparisons for different levels of temperature be independent of time.

A similar situation arises if all of the tests in a factorial design are made, but some of the tests are not made as many times as the other tests. Procedures have been devised for evaluating data from some types of nonorthogonal experiments, but they are more complex than procedures for evaluating orthogonal data. In some instances the missing values can be estimated from the data available so that the advantages of orthogonality can be used in approximate methods of analysis.

There are designs that are orthogonal even though all tests are not made the same number of times. Consider a factorial experiment to study the effects of two factors,  $X_a$  and  $X_b$ . The estimates of the various effects will be independent if the number of replicates of each test made at any level of factor  $X_a$  is a constant multiple of the number of replicates of each corresponding test made at any other level of factor  $X_a$ . For example, suppose both factors are studied at three levels. The tests at the first level of factor  $X_a$  may each be made once, those at the second level twice, and those at the third level three times. Similarly, the tests at the first, second, and third levels of factor  $X_b$  may each be made twice, once, and three times, respectively. These two ratios for the levels of factor  $X_a$  and the levels of factor  $X_b$  may be incorporated into a single experiment. The following array gives the number of replicates to be made for each test in the two-factor, three-level factorial design:



Level of factor $X_a$	Level of factor $X_b$			
	1	2	3	
1:	2	1	3	(140)
2:	4	2	6	
3:	6	3	9	

A design which includes proportional replication of the kind illustrated in the array (140) is orthogonal and is useful when the magnitude of experimental error varies from one factor level to another. This application also is discussed in the section on the importance of experimental error in design considerations. The more common design in which all tests are made the same number of times is simply a special case of proportional replication.

### Two-Level Factorial Designs

Factorial designs in which two levels are selected for each factor are particularly applicable in the conduct of preliminary research and in the determination of optimum operating conditions. Suppose a standard procedure were used to leach a copper ore at 25 percent solids for 30 minutes at 25° C. The question arises as to whether a better set of leaching conditions can be found for this particular ore. Three factors which may be varied are  $X_a$ , percent solids;  $X_b$ , leaching time; and  $X_c$ , leaching temperature. For purposes of illustration, the second levels for each factor may be chosen to be 35 percent solids, 40 minutes, and 35° C. There is a good chance for interactions to exist between these factors; a higher percent solids may require longer leaching time, a higher temperature may reduce the time necessary to obtain optimum copper extraction, and so on. A full two-level factorial design to estimate the three main effects and four possible interaction effects consists of eight tests. The results of these eight tests will give estimates of the relative magnitudes of the various effects. If an estimate of experimental error were available, the results would show which of the effects are important enough for further investigation.

It may be desirable to explore a larger range of values for each of the factors in this experiment, say 15 to 45 percent solids, 10 to 60 minutes' leaching time, and 15° to 90° C. The set of eight tests in the two-level factorial design previously described can be the first step in an exploration of the larger region. Evaluation of the results of this set will show how to vary the three factors simultaneously to find the optimum leaching conditions within the region. The results may show, for example, that starting with the central value of each factor in the initial, two-level, factorial design the optimum conditions will be approached most rapidly if the percent solids is increased by 7 percent and time is increased by 4.5 minutes for each temperature increase of 10° C. The procedure is outlined as follows: A set of tests is made, evaluation of the data from this set determines another set of tests to be made, evaluation of the data from the second set determines still another set, and the procedure is continued until the optimum conditions are located in the region. It is possible to locate the optimum conditions with more certainty and with fewer tests in this way than by the one-factor-at-a-time approach.

To develop a single method for analyzing the results of factorial experiments regardless of particular levels selected for the various factors, it is necessary to define the concepts of base level and design unit for each factor in an experiment. The base level for each factor in a two-level factorial design is the average level of that factor. Therefore, the base levels in the initial two-level factorial leaching experiment are 30 percent solids, 35 minutes' leaching time, and 30° C. leaching temperature. The design unit for each factor in a two-level experiment is the difference between the higher and lower levels. The design units in the leaching experiment are 10 percent solids, 10 minutes, and 10° C. The use of these concepts corresponds to the translation of coordinate axes of the response function from the natural origin at 0 percent, 0 minutes, and 0° C. to the base levels of each factor, and to the change in scale from natural units to design units. The lower level of each factor is simply one-half a design unit below the base level, and the higher level is one-half a design unit above the base level. These concepts form the basis for subsequent discussions of factorial designs and the analysis of results obtained. The relative locations of the various tests in the three-factor two-level factorial design are shown geometrically in figure 8. In this figure, the lower levels,  $-1/2$ , represent 25 percent solids for  $X_a$ , 30 minutes' leaching time for  $X_b$ , and 25° C. leaching temperature for  $X_c$ . The higher levels,  $+1/2$ , represent 35 percent, 40 minutes, and 35° C., respectively, for  $X_a$ ,  $X_b$ , and  $X_c$ . Each design point is identified by the test symbol, the coordinates of the point in design units, and the response obtained from the test at the point. In the discussion and illustration of two-level factorial designs, the subscripts are omitted from the test symbols.

The various main and interaction effects of the three factors upon the amount of copper leached are estimated by means of appropriate differences in the responses obtained under different test conditions. For two-level factorial designs, each main and interaction effect that can be estimated has only one polynomial component. Hence, in two-level designs, one may speak of the coefficient of an effect, instead of the coefficient of a component of the effect. For example, the estimated coefficient A of the linear main effect of percent solids is equal to the difference between the average response for the four tests at 35 percent and the average response for the four tests at 25 percent; that is,

$$A = (1/4)(y_{211} + y_{212} + y_{221} + y_{222}) - (1/4)(y_{111} + y_{112} + y_{121} + y_{122}). \quad (141)$$

If there were no interaction effect between percent solids and leaching time, estimates obtained from tests made at the higher and lower levels of time should be equal. When such an interaction exists, the corresponding coefficient AB will be equal to one-half the difference between the two estimates; that is,

$$\begin{aligned} AB &= (1/2)[(1/2)(y_{221} + y_{222} - y_{121} - y_{122}) \\ &\quad - (1/2)(y_{211} + y_{212} - y_{111} - y_{112})] \\ &= (1/4)[y_{221} + y_{222} + y_{111} + y_{112} \\ &\quad - (y_{121} + y_{122} + y_{211} + y_{212})]. \end{aligned} \quad (142)$$

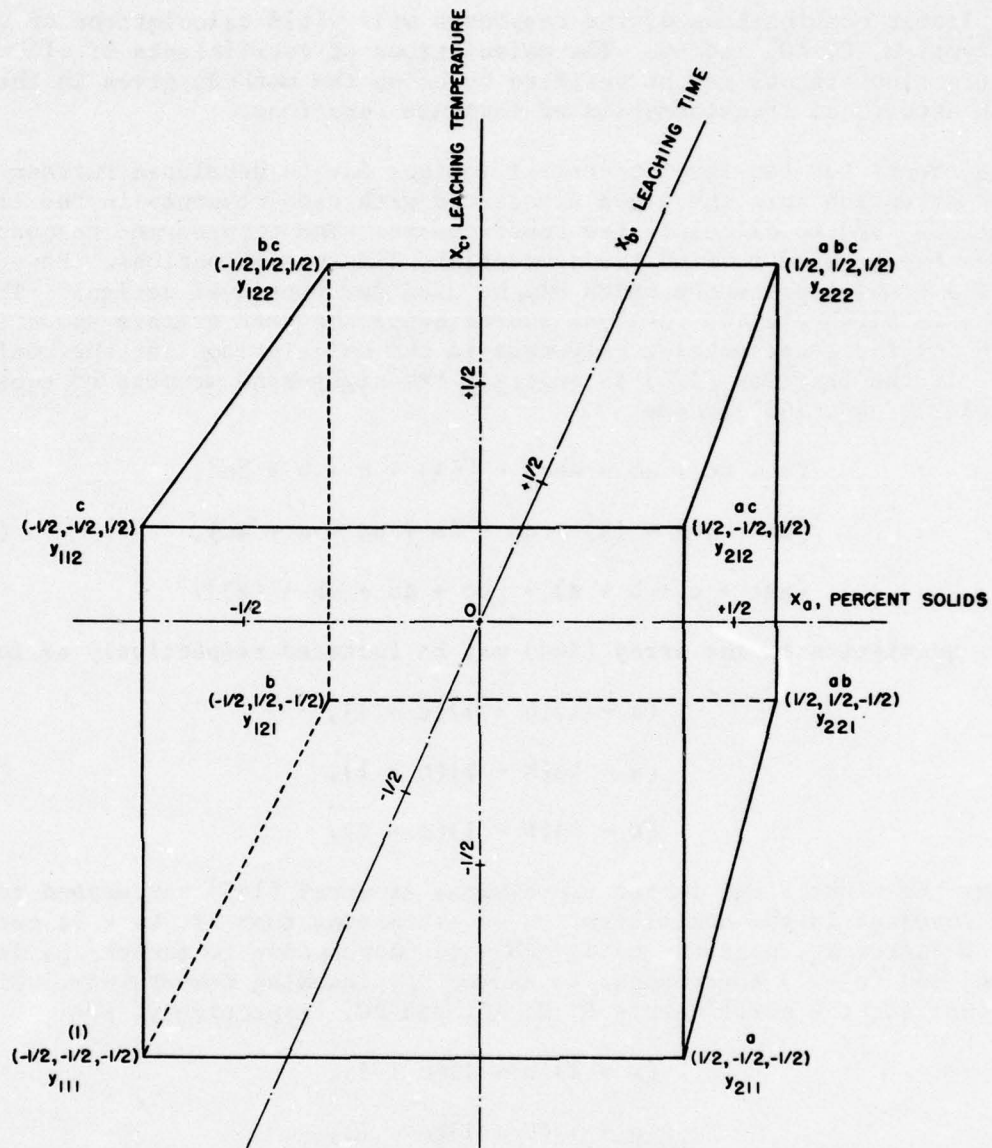


FIGURE 8. - Diagram of a Two-Level Factorial Design for Three Factors.

The coefficient ABC of the three-factor interaction effect of percent solids, time, and temperature is equal to one-half the difference between two estimates of the coefficient AB obtained from tests made at the higher and lower levels of temperature; that is,

$$\begin{aligned}
 ABC &= (1/2)[(1/2)(y_{222} + y_{112} - y_{122} - y_{212}) \\
 &\quad - (1/2)(y_{221} + y_{111} - y_{121} - y_{211})] \\
 &= (1/4)[(y_{222} + y_{112} + y_{121} + y_{211}) \\
 &\quad - (y_{122} + y_{212} + y_{221} + y_{111})].
 \end{aligned}
 \tag{143}$$



Similar linear combinations of the responses will yield calculations of the coefficients B, C, AC, and BC. The calculations of coefficients of all main and interaction effects may be verified by using the methods given in the sections on orthogonal transformation of response functions.

The theory for two-level factorial designs may be developed further by focusing attention upon the signs associated with each response in the linear combinations used to calculate the coefficients. The transformed response functions may be used to find the appropriate linear combinations. However, there is a simpler procedure which may be used for two-level designs. The procedure is algebraic and involves substituting the test symbols shown in figure 8 for the corresponding responses in the calculations for the coefficients. If the fraction (1/4) is omitted, the right-hand members of equations (141), (142), and (143) become

$$\begin{aligned}(a + ac + ab + abc) - [(1) + c + b + bc], \\ [ab + abc + (1) + c] - (b + bc + a + ac), \\ (abc + c + b + a) - [bc + ac + ab + (1)].\end{aligned}\tag{144}$$

The quantities in the array (144) may be factored respectively as follows:

$$\begin{aligned}(a - 1)(b + 1)(c + 1), \\ (a - 1)(b - 1)(c + 1), \\ (a - 1)(b - 1)(c - 1).\end{aligned}\tag{145}$$

Note that the minus signs in the expressions of array (145) correspond to the factors involved in the coefficient to be estimated; that is, (a - 1) corresponds to factor  $X_a$ , percent solids; (b - 1) corresponds to factor  $X_b$ , leaching time; and (c - 1) corresponds to factor  $X_c$ , leaching temperature. Similar expressions for the coefficients B, C, AC, and BC, respectively, are

$$\begin{aligned}(a + 1)(b - 1)(c + 1), \\ (a + 1)(b + 1)(c - 1), \\ (a - 1)(b + 1)(c - 1), \\ (a + 1)(b - 1)(c - 1).\end{aligned}\tag{146}$$

Therefore, in the general case expressions similar to those in arrays (145) and (146) may be set up with minus signs corresponding to the factors involved in the coefficient to be estimated, and then those expressions expanded to obtain the proper signs for the tests as shown in the expressions of array (144). The same signs then are used in the linear combinations of the corresponding responses which are used to calculate the coefficients.

The signs to be associated with the responses for the various tests when calculating the coefficients for the three-factor, two-level, factorial copper leaching experiment are summarized in table 5. Tables of this kind are useful in designing two-level fractional factorial experiments, and for this reason the column for the average effect coefficient, I, is included. The upper left-hand corner of the table can be used for a two-factor experiment. The table can be extended for use with four or more factors.<sup>8</sup>

TABLE 5. - Signs to be associated with the responses for the tests in a three-factor, two-level, factorial experiment when calculating the coefficients of the main and interaction effects for the factors  $X_a$ ,  $X_b$ , and  $X_c$

Test No.	Coefficient							
	I	A	B	AB	C	AC	BC	ABC
(1)	+	-	-	+	-	+	+	-
a	+	+	-	-	-	-	+	+
b	+	-	+	-	-	+	-	+
ab	+	+	+	+	-	-	-	-
c	+	-	-	+	+	-	-	+
ac	+	+	-	-	+	+	-	-
bc	+	-	+	-	+	-	+	-
abc	+	+	+	+	+	+	+	+

To understand how the table is extended for more factors, notice the signs in columns A, B, and C. The minus sign in column A corresponds to a test in which factor  $X_a$  is at its lower level, and the plus sign corresponds to a test in which factor  $X_a$  is at its higher level. The same is true for columns B and C and the factors  $X_b$  and  $X_c$ , respectively. For each test, the signs in columns A, B, and C agree with the signs of the coordinates of the test point in figure 8. The sign in column AB for any row is the product of the signs for that same row in columns A and B. The signs in columns AC, BC, and ABC are found in the same way.

To extend the table for a fourth factor,  $X_d$ , the test symbols for the three-factor factorial design in the left column are each multiplied by the letter d, that is, d, ad, bd, abd, cd, acd, bcd, and abcd. Eight additional rows are added to the table corresponding to these additional test symbols in

<sup>8</sup>Davies, O. L., Design and Analysis of Industrial Experiments: Hafner Publishing Co., New York, N.Y., 1956, table M, p. 624a.



the order given. Similarly, the coefficient symbols at the head of the remaining columns are each multiplied by the letter D to give D, AD, BD, ABD, CD, ACD, BCD, and ABCD.<sup>9</sup> Eight additional columns corresponding to these additional coefficients are added to the table in the order given. The signs in the eight new rows for the first eight columns of the extended table will be the same, respectively, as the signs in the eight rows of table 5, that is, row d will be the same as row (1), row ad will be the same as row a; and so on. Minus signs are placed in the first eight rows of column D of the extended table, and plus signs are placed in the last eight rows of this column. The signs in the remaining seven added columns are obtained as products of the appropriate corresponding signs in columns A, B, C, and D as previously explained for table 5. The table may be successively extended in a similar way for any number of factors.

If one of the factors in a two-level experiment were qualitative instead of quantitative, then either level of that factor would be selected as the lower level and considered to be one-half a design unit below an artificial base level. The other level then is considered to be the higher level, one-half a design unit above the artificial base level. The effect of the qualitative factor has one artificial linear component for which the corresponding coefficient may be calculated from the results of a two-level factorial experiment. Similarly, interaction effects involving one or more qualitative factors may be considered to have corresponding artificial polynomial components.

#### Factorial Designs With More than Two Levels per Factor

Factorial designs in which more than two levels are selected for some or all of the factors are used when a more complete investigation of the relationships between factors and responses is desired. Two-level factorial designs can be used to explore a region only when the main effects of the factors are linear or approximately linear over the region, and interaction effects are relatively small compared to the main effects. However, when main effects are not linear over the region of interest and interaction effects are relatively large, more than two levels for the factors are necessary for a complete study of the response surface.

Typical experiments wherein the factors must be tested at more than two levels are illustrated as follows: An oxidized nickel ore is subjected to a reducing roast to convert the metal oxide to metal. At 600° and 700° C. roasting temperature, 80 and 82 percent of the nickel, respectively, are converted to metallic form. Comparison with an available estimate of experimental error shows this difference to be insignificant. There may be several explanations for these results: (1) The maximum possible reduction may have been obtained, (2) a still higher temperature may be necessary to break down certain compounds in the ore which represent 18 to 20 percent of the metal, or (3) side reactions at 700° C. may cause some of the reduced metal to

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<sup>9</sup>Note: (1)d = d and ID = D. Multiplication of test and coefficient symbols is discussed more fully in the section on group theory methods for fractional factorial designs.



recombine with other materials present. In the absence of additional information about the reactions involved, it is possible that a higher percent reduction might be obtained either at 650° or at 800° C. If such possibilities are suspected in advance, the original experimental design should include at least three levels for temperature.

Now, suppose a second factor, time, also is to be studied at the levels 1 and 2 hours. The four tests in a two-level factorial experiment may be test (1): 600° C., 1 hour; test a: 800° C., 1 hour; test b: 600° C., 2 hours; and test ab: 800° C., 2 hours. The results for tests (1), a, and b may be 89, 90, and 87 percent reduction, respectively. Either the increase in temperature or in time appears to yield an increase in percent reduction. However, the result for test ab is only 83 percent reduction. If experimental error were less than, say, 1 percent, such a result would be evidence of an important interaction effect between time and temperature. The design should be expanded to include a third level for each factor, say 700° C. and 1.5 hours, to further evaluate the effects.

If there were evidence to indicate that a response has a maximum value at some interior point in an experimental region and has lower values around the boundary of that region, it would be necessary in locating the maximum value to include at least three levels for each factor in a design which covers the region. The success in locating the maximum value by using a specific number of levels will depend upon the relative importance of the higher order components that are not estimated by the design. In the procedure for determining optimum conditions for a process, the response values obtained may increase to a point and then begin to decrease again. In the neighborhood of such a point, a factorial design with at least three levels per factor must be used to estimate quadratic components of the main effects of the factors and pinpoint the optimum conditions.

The base levels and design units for factorial experiments of three levels or more are defined in a manner similar to that for two-level designs. The base level for a factor is always the average value of the factor levels in the design in terms of the original factor units. The design unit is the difference between two adjacent levels. Therefore, in a roasting experiment to study the effect of temperature at 600°, 700°, and 800° C., the base level is 700° C. When the effect of time is to be studied at 1, 2, 3, and 4 hours, the base level is 2.5 hours. The corresponding design units in these examples are 100° C. and 1 hour, respectively. The levels of each factor are equally spaced; otherwise, the discussion of the design and subsequent analysis of results is more complicated. In a specific research problem, it might be preferable to study the effect of temperature by using equal spacing of values of the function  $e^T$  in the design, instead of equal spacing of  $T$  values, and to make similar transformations of the units of other factors. The base levels and design units then are defined in terms of the transformed variables.

The general procedures for calculating the estimated coefficients of the various effect components for factorial experiments are given in the sections on orthogonal transformation of response functions. Tables of signs to be associated with the responses for the various tests are not prepared for

designs involving three or more levels per factor. There are only two algebraic signs, and the convenience of associating one sign with each level of a factor is lost.

The factors in the previous examples are quantitative. It also is possible to test for effects of qualitative factors in the same way. One qualitative factor which often is studied in metallurgical research is the type of acid to be used for leaching, and two levels which may be selected are hydrochloric acid and sulfuric acid. In this case, the concepts of base level and design unit have no physical meaning, but procedures to evaluate the main and interaction effects involving qualitative factors are the same as for quantitative factors. The only exception is that if three or more levels are selected for a qualitative factor, the linear, quadratic, and higher order components of the effects have no physical meaning. Therefore, only the overall effects are estimated.

#### Fractional Factorial Designs and Confounding

It is not always practical or necessary to make all the tests in a full factorial design. As the number of factors to be tested in an experiment increases, the number of tests in a full factorial design increases rapidly. If some of the interaction effects are insignificant, it may be possible to reduce the number of tests in a design by combining the estimates of the various effects so that only the important effects need be studied in an experiment. When the estimates of effects thus are combined, they are said to be confounded.

Fractional factorial designs and the principle of confounding are particularly useful when it is necessary to introduce minor factors into an experiment. Such factors are of no interest in themselves, but it is important to plan the experiment so that the effects of these minor factors do not interfere with the estimates of the effects of major experiment factors. For example, a two-level factorial experiment to study the effects of four physico-chemical factors requires 16 tests. To obtain estimates of the desired effects, the other experiment conditions must be constant. This may be impossible, particularly if the tests of the experiment must be made in two or more sets on different days or by different men so as to complete the entire experiment in 1 day. In designing experiments involving uncertainty about control of minor factors, the number of tests to be made is not changed, but the manner in which the tests are divided into blocks should be planned so that any effect due to making the tests in different blocks will not be confounded with important effects of the major factors being tested.

A two-level leaching experiment may be designed to study the effects of time,  $X_a$ , at 1 and 2 hours; temperature,  $X_b$ , at 25° and 50° C.; type of acid,  $X_c$ , using hydrochloric and sulfuric acids, and concentration of acid,  $X_d$ , at 50 and 100 grams per liter in the leach solution. There are 16 tests in the full replicate of this design, and the results of such an experiment may be used to calculate the coefficients A, B, C, D, AB, AC, AD, BC, BD, CD, ABC, ABD, ACD, BCD, and ABCD. Suppose two men each make eight of the tests, all tests at 25° C. are made by one man, and all tests at 50° C. are made by the



other man. If there were any difference in the performance of the two men, the effects of the difference in performance upon the response, in this instance, metal extraction, would be confounded with the effect of temperature. The only valid conclusion which can be drawn from the results obtained is that the coefficient B in this case is due either to temperature or the difference in performance of the two men or both factors. Only if it were known that the performances of the two men are essentially the same would the coefficient B be attributed to temperature. However, it may not be convenient to plan and conduct an experiment to compare the performances of the two men before conducting the main leaching experiment. The effect of a difference in performance can be confounded with one of the less important interaction effects instead of with the main effect of temperature as in the above example.

#### Method of Confounding Effects by Table of Signs

The procedures for confounding effects in fractional factorial designs are based on the principles of mathematical group theory. Before describing the general procedures for confounding effects, the method involving use of a table of signs will be illustrated. This method can be used for two-level designs because a minus sign can be associated with the lower level and a plus sign with the higher level of each factor. The method based upon a table of signs cannot be used if any factors are to be tested at more than two levels. Later, the procedure for confounding will be presented in a more general and more abstract way for use with designs in which the factors are tested at any number of levels.

The method of confounding by the use of signs now is illustrated for a three-factor experiment with a two-level design in which it is necessary to estimate the main effects of factors  $X_a$ ,  $X_b$ , and  $X_c$  and in which all interactions between the three factors are nonexistent or negligible. In a typical instance factor  $X_c$  may be the necessary result of investigating factors  $X_a$  and  $X_b$  in two blocks of tests due to limitations of equipment, time, or personnel. The first step is to construct a table of signs to be associated with the responses for the tests when calculating the coefficients of the various effect components. Such a table is illustrated in table 5. The second step is to select four of the eight tests in table 5 so that the main effect of the block factor  $X_c$  is confounded with the interaction effect between time,  $X_a$ , and temperature,  $X_b$ . This is accomplished by selecting those tests from table 5 for which the sign in column AB is the same as the sign in column C. These tests and their signs then are incorporated in a second table as shown in table 6. The first two tests are made at the lower level of factor  $X_c$ , and the last two tests are made at the higher level; that is, tests a and b are made in the first block, and tests c and abc are made in the second block.

TABLE 6. - Tests selected from the eight tests of a three-factor, two-level, factorial experiment in such a way that the interaction coefficient AB is confounded with the main coefficient C

Test symbol	Coefficient							
	I	A	B	AB	C	AC	BC	ABC
a	+	+	-	-	-	-	+	+
b	+	-	+	-	-	+	-	+
c	+	-	-	+	+	-	-	+
abc	+	+	+	+	+	+	+	+



Whenever the tests of a full factorial design are selected so as to confound two particular effects, all effects will be confounded in pairs. Table 6 illustrates the confounding of the effects whose coefficients are AB and C. A study of the table shows that the effects whose coefficients are B and AC also are confounded. The same is true of the effects whose coefficients are A and BC and of those whose coefficients are I and ABC. The nature of the minor factors which cause block effects is such that only the main effects are considered to be important. The metallurgist must be careful to conduct an experiment so as to minimize such effects, and the principle of confounding may be used as a precaution against anticipated or unforeseen variations in test conditions. In this illustration the interaction effects between blocks and the major experiment factors, time and temperature, and the corresponding coefficients AC, BC, and ABC are negligible. However, in the more general case, it is necessary to study the complete system of confounding which results when two effects, or their coefficients, are selected to be confounded.

To show further how the effects and their corresponding coefficients are confounded by selecting the four tests in table 6, let particular factor levels for factors  $X_a$ ,  $X_b$ , and  $X_c$  be identified by the letters i, j, and k, respectively. The response function for a three-factor, two-level experiment then will be

$$\begin{aligned}\bar{y}_{ijk} &= IZ_{000}(ijk) + AZ_{100}(ijk) + BZ_{010}(ijk) + CZ_{001}(ijk) + ABZ_{110}(ijk) \\ &\quad + ACZ_{101}(ijk) + BCZ_{011}(ijk) + ABCZ_{111}(ijk) \\ &= I \pm \frac{1}{2}A \pm \frac{1}{2}B \pm \frac{1}{2}C \pm \frac{1}{2}AB \pm \frac{1}{2}AC \pm \frac{1}{2}BC \pm (1/8)ABC.\end{aligned}\quad (147)$$

If each test in table 6 were made once, the average response  $\bar{y}_{ijk}$  for each test would be the single response  $y_{ijk}$  obtained. The terms in equation (147) may be rearranged for the four tests a, b, c, and abc, respectively, to give the following algebraic sums:

$$\begin{aligned}y_{a11} &= [I + (1/8)ABC] + (\frac{1}{2}A + \frac{1}{2}BC) - (\frac{1}{2}B + \frac{1}{2}AC) - (\frac{1}{2}C + \frac{1}{2}AB), \\ y_{1a2} &= [I + (1/8)ABC] - (\frac{1}{2}A + \frac{1}{2}BC) + (\frac{1}{2}B + \frac{1}{2}AC) - (\frac{1}{2}C + \frac{1}{2}AB), \\ y_{11a2} &= [I + (1/8)ABC] - (\frac{1}{2}A + \frac{1}{2}BC) - (\frac{1}{2}B + \frac{1}{2}AC) + (\frac{1}{2}C + \frac{1}{2}AB), \\ y_{2a22} &= [I + (1/8)ABC] + (\frac{1}{2}A + \frac{1}{2}BC) + (\frac{1}{2}B + \frac{1}{2}AC) + (\frac{1}{2}C + \frac{1}{2}AB).\end{aligned}\quad (148)$$

Now the four responses and their equalities in the equation set (148) may be combined algebraically to calculate

$$C + \frac{1}{2}AB = \frac{1}{2}(-y_{a11} - y_{1a2} + y_{11a2} + y_{2a22}).\quad (149)$$

Since the data from the four tests cannot be used to calculate C and AB separately, but only the sum,  $C + \frac{1}{2}AB$ , the two coefficients are said to be confounded with each other. The three other sums of confounded coefficients which may be calculated from the data are

$$I + (1/8)ABC, A + \frac{1}{2}BC, \text{ and } B + \frac{1}{2}AC.\quad (150)$$

The half replicate of a three-factor, two-level, factorial design that consists of the block of four tests in table 6 is an adequate design if at least one of the coefficients in each sum is known to be negligible. The second coefficient in each pair in the set of sums (150) is an interaction coefficient involving factor  $X_C$ . As no interaction effects exist between different blocks of tests and the experiment factors time and temperature, the second coefficient in each pair may be considered to be equal to zero. The corresponding algebraic combinations of the responses, therefore, may be set equal to the first coefficient in each pair. If the coefficient AB were negligible for the range of levels selected for each factor, the coefficient C might be calculated.

The other block, which can be used for the experiment to give the same system of confounding, is the half replicate consisting of the four remaining tests in table 5, that is, tests (1), ab, ac, and bc. These could have been found first by selecting those tests in table 5 which have opposite signs in columns AB and C. In this case, four algebraic combinations of the responses may be obtained which are equal to

$$C - (1/2)AB, I - (1/8)ABC, A - (1/2)BC, \text{ and } B - (1/2)AC. \quad (151)$$

When these assumptions are valid, either the four tests in table 6 or this second block of four tests may be made to obtain calculations of the desired coefficients.

Coefficients that are confounded with each other in a fractional factorial design are called aliases. Therefore, in either of these designs consisting of four tests, the coefficients C and AB are aliases, the coefficients I and ABC are aliases, and so on. In general, a two-level factorial experiment to investigate  $n$  factors contains  $2^n$  tests, and the responses obtained can be used to calculate the average effect coefficient I and  $(2^n - 1)$  coefficients of the possible components of the factor effects. These  $2^n$  coefficients all will be confounded in pairs of aliases whenever a half replicate of such an experiment is designed. The value of such designs depends upon the ability to select tests in such a way that no two important coefficients will be confounded with each other.

More complex systems of confounding can be used to reduce the number of tests necessary for an investigation if interaction effects of major factors are negligible. For example, if five factors are to be tested and all interaction effects are known to be negligible, only the main effect of each factor needs to be estimated. The full two-level factorial design for five factors contains 32 tests. The eight tests in a quarter-replicate design may be selected in such a way that algebraic combinations of responses may be used to calculate the following sums of aliases:



$$\begin{aligned}
& I + (1/8)ABD + (1/8)ACE + (1/16)BCDE, \\
& A + (1/2)BD + (1/2)CE + (1/16)ABCDE, \\
& B + (1/2)AD + (1/8)ABCE + (1/4)CDE, \\
& C + (1/8)ABCD + (1/2)AE + (1/4)BDE, \\
& D + (1/2)AB + (1/8)ACDE + (1/4)BCE, \\
& E + (1/2)AC + (1/8)ABDE + (1/4)BCD, \\
& DE + BC + (1/2)ABE + (1/2)ACD, \\
& BE + CD + (1/2)ABC + (1/2)ADE.
\end{aligned} \tag{152}$$

The six coefficients  $I$ ,  $A$ ,  $B$ ,  $C$ ,  $D$ , and  $E$  are calculated from the responses of the eight tests selected. Also, since all interaction effects are negligible, the algebraic combinations of responses that give the last two sums of aliases can be used for an estimate of experimental error.

Such a design also may be used when it is necessary to divide the tests of a factorial design into four blocks of tests. For example, a two-level factorial design for the four factors  $X_a$ ,  $X_b$ ,  $X_c$ , and  $X_d$  requires 16 tests. Now, suppose the required tests must be made in four blocks of four tests each. The effects of making the tests in four different blocks may be treated as the effects of two additional factors  $X_e$  and  $X_f$ , each at two levels. The 16 tests then become a quarter replicate of a six-factor, two-level experiment.

The only important effects involving blocks will correspond to the main effect coefficients  $E$  and  $F$  and the interaction effect coefficient  $EF$ . The experiment may be designed so that important coefficients of the original four factors will not be confounded with  $E$ ,  $F$ , or  $EF$ . This may be accomplished by first constructing a table of signs for a full six-factor, two-level, factorial experiment by procedures discussed in the section on two-level designs. From this table, 32 tests may be selected that will confound coefficient  $E$  with an unimportant interaction coefficient for the experiment factors  $X_a$ ,  $X_b$ ,  $X_c$ , and  $X_d$ . From the table of 32 tests and their signs so obtained, a selection of 16 tests can be made so as to confound coefficient  $F$  with another unimportant interaction coefficient for the four experiment factors.

#### General Methods for Confounding Effects

The method of confounding by means of a table of signs is relatively simple, but it is limited to two-level designs. Also, the method becomes rather cumbersome as the number of factors increases and as the confounding becomes more complex. The general procedure for determining the tests to be made to confound effects in a fractional factorial design may appear highly abstract to the reader who is not familiar with mathematical group theory. A short discussion of group theory, therefore, will be presented before describing how the general procedure is employed. Once the basic principles of group theory are understood, the general procedure is more readily applied than the method based upon a table of signs.

Group Theory. - A group is defined mathematically to be a set of elements together with an operation defined in such a way that whenever the operation is performed with two elements in the set, the result is another element in the set. In addition, there must be an identity element in the set such that



when the operation is performed with the identity element and any second element, the result leaves the second element unchanged. Finally, for each element in the set, there must be a second element such that when the operation is performed with these two elements, the result is the identity element. These two elements are called inverses of each other. For example, the set of all positive and negative whole numbers and the operation, addition, constitute a group. The numbers 5 and 19 are integers and  $5 + 19 = 24$ , also an integer. Similarly,  $7 + (-9) = -2$ . The identity element in this case is 0, for example  $0 + 7 = 7$ . The inverse of an integer, say 5, is -5, that is,  $5 + (-5) = 0$ . There are an infinite number of elements in this group. Similarly, the set of all rational numbers and the operation, multiplication, also form a group with an infinite number of elements. The number zero has no inverse under multiplication, but if all other elements in a set have inverses within the set, the set together with the operation, multiplication, is a group.

An example of a group with a finite number of elements is the set of two elements, +1 and -1, and the operation, multiplication. The structure of this finite group is illustrated as follows:

.	+1	-1
+1	+1	-1
-1	-1	+1

(153)

The identity element, +1, for the group is listed first in the column headings and in the row headings. The remaining values in the table are the products of the corresponding row and column elements. The dot in the upper left-hand corner indicates the operation, multiplication. Each element in this group is its own inverse. A group having two elements but a different structure from that shown in group (153) consists of the integers zero and 1 and the operation, multiplication. Again the identity element for multiplication is 1, and it is listed first.

.	1	0
1	1	0
0	0	0

(154)

The concept of integers modulo  $k$  is a mathematical concept which is useful in the study of group theory. The concept may be introduced by considering the measure of time in cycles of 12 hours. Nine hours after midnight it is 9 o'clock. However, 5 hours later, it is not 14 o'clock, but 2 o'clock. Another 11 hours later, it is not 25 o'clock, but 1 o'clock. The above statements may be expressed symbolically as follows:  $9 + 5 = 2$ ,  $9 + 5 + 11 = 1$ . If midnight and noon are designated by zero instead of 12, the hours of the clock represent the integers modulo 12. These integers and the operation, addition, constitute a finite group. If any two or more of the integers from zero through 11 are added in this manner, the result also is one of these

integers. The identity member of this group is zero, and the additive inverse of any other member is the difference between 12 and that member. For example,  $5 + 7 = 0$ ; in other words, 7 hours after 5 o'clock, it is either noon or midnight. In general, the integers modulo  $k$  are those integers in the set  $0, 1, 2, \dots, (k-1)$ .

The integers modulo 2 and the operation, addition, constitute a group with the structure shown as follows:

+	0	1
0	0	1
1	1	0

(155)

The identity element in this case is zero, and each element is its own inverse. The structure of arrangement (155) is the same as that shown in arrangement (153). This means that both elements in each group are found in the same relative locations in each arrangement. It is the structure of this group, whether expressed as in arrangement (153) or (155), which forms the basis of the method of confounding by means of a table of signs.

The structure of the group consisting of the integers modulo 4 and the operation, addition, is as follows:

+	0	1	2	3
0	0	1	2	3
1	1	2	3	0
2	2	3	0	1
3	3	0	1	2

(156)

The identity element is zero, and the inverse of each element is the difference between 4 and that element. The structure of this group is illustrated by the relative locations of each element in the arrangement (156). It has been shown that the group consisting of the integers modulo 2 and addition and having the structure illustrated in the arrangement (155) has the same structure as the group consisting of the two numbers, +1 and -1, and multiplication which has the structure illustrated in the arrangement (153). Similarly, the group consisting of the integers modulo 4 and addition will be shown to have the same structure as a group defined for the coefficients  $I, A, A^2$ , and  $A^3$  for a one-factor, four-level experiment. However, before illustrating this relationship, it is necessary to define a new concept, group theory multiplication. The operation is used to obtain products of coefficients and thereby to determine which coefficients are aliases in a fractional factorial design.

In this case the products of two or more coefficients are purely symbolic and do not refer to the numerical values of the coefficients involved. When

two different coefficients are set equal to each other, the equal sign represents the expression "is confounded with." In a four-level experiment, the coefficient  $A^4$  is confounded with coefficient I. Therefore, the symbolic statement,  $A^4 = I$ , serves to define the properties of group multiplication for this experiment. With this definition, the product of any coefficients will be one of the four coefficients I, A,  $A^2$ , and  $A^3$ . Coefficient I serves as the identity element in the group. Therefore,  $A(A^2) = A^3$ ,  $A(A^3) = I$ ,  $A^2(A^3) = AI = A$ , and so on. The inverse of any element  $A^i$  is  $A^{4-i}$ , where  $i = 1, 2, 3$ ; for example,  $A(A^3) = I$ . The four coefficients and the group multiplication operation constitute a finite group with the following structure:

.	I	A	$A^2$	$A^3$	
I	I	A	$A^2$	$A^3$	
A	A	$A^2$	$A^3$	I	(157)
$A^2$	$A^2$	$A^3$	I	A	
$A^3$	$A^3$	I	A	$A^2$	

Note that the relative locations of the powers  $i$  of A in the group (157) are the same as the relative locations of the integers modulo 4 in the group (156). The two groups have the same structure.

**Group Theory in Design.** - The principles of group theory form the basis for the general procedure for confounding effects in fractional factorial designs. The groups of primary interest are those which consist of sets of coefficients which are calculated from the results of full factorial experiments and the group theory multiplication operation extended for use in experiments having more than one factor.

The application of group theory principles to the design of fractional factorial experiments is presented first in the following discussion in terms of two-level designs. Two-level factorial experiments are designed to estimate linear components of the main effects of the factors and the corresponding components of the interaction effects. Such designs cannot be used to estimate quadratic components of the main effects. An application of the method of confounding based upon a table of signs would show that all main effect quadratic component coefficients are confounded with each other and with the average effect coefficient I in a two-level design. This is expressed in the symbolic notation of group theory as follows:

$$A^2 = B^2 = C^2 = D^2 = \dots = I. \quad (158)$$

Because of this confounding, the symbolic product of coefficients obtained by group multiplication results in a product that is one of the coefficients for which a two-level experiment is designed. For example,  $(AB)(AC) = A^2BC$ ; however,  $A^2$  is confounded with I which serves as the identity and is omitted from any product unless it stands alone. Therefore,  $(AB)(AC) = BC$ .



A four-factor, two-level experiment will be used to illustrate the use of group theory for the design of a half replicate of the corresponding full factorial design. The 16 coefficients which are calculated from the results of the full replicate design are I, A, B, C, D, AB, AC, AD, BC, BD, CD, ABC, ABD, ACD, BCD, and ABCD. These constitute the set of elements in the group that are to be confounded in pairs in a half-replicate design. The identity element in this group is the coefficient I. For two-level designs, each coefficient is its own inverse. Suppose D were to be confounded with ABC; that is,  $D = ABC$  in group theory notation. The first step toward finding the other pairs of aliases is to determine which coefficient is confounded with I as a consequence of the decision to confound D with ABC. If both sides of the expression  $D = ABC$  are multiplied by the same element, the symbolic equality is preserved. Therefore,  $D^2 = ABCD$ , but  $D^2$  is confounded with I according to the defining expression (158), and so  $I = ABCD$ . After determining that I is confounded with ABCD, these two coefficients may be multiplied by any other coefficient to find its alias. For example,  $AI = A^2BCD$ , or  $A = BCD$ . The 16 coefficients are found to be confounded in pairs of aliases as follows:

$$\begin{array}{ll}
 D = ABC & C = ABD \\
 I = ABCD & AB = CD \\
 A = BCD & AC = BD \\
 B = ACD & AD = BC
 \end{array} \quad (159)$$

Any pair of coefficients in the set of pairs (159) could have been chosen initially, and the results would have been the same. For example, if the initial decision had been to confound AB with CD; that is,  $AB = CD$ , then the first step would be to find the alias of I by multiplying either AB or CD by itself, for example,  $(AB)(AB) = (AB)(CD)$ . The product  $(AB)(AB) = A^2B^2$ ; both  $A^2$  and  $B^2$  are confounded with I, and so  $A^2B^2 = I^2$ . The operation of the identity, I, upon itself leaves it unchanged, so  $I^2 = I$ , and  $I = ABCD$ . Then the other pairs of aliases would be found just as before.

As a second example, an experiment may be designed to study the effects of several factors upon metal reduction during roasting. Two quantitative factors to be studied are residence time,  $X_a$ , and roasting temperature,  $X_b$ . The reliability of the results obtained depends upon the accuracy of analytical procedures used to assay the calcines produced, so a qualitative factor,  $X_c$ , is included in the design to study two different types of chemical analysis. A fourth factor,  $X_d$ , is included to study the effects of two different types of ore used in the tests. It may be known or assumed that the coefficient AC of the interaction between the residence time in the furnace and the type of chemical analysis used to assay the calcine is negligible, and so one may wish to confound D with AC. Then  $D^2 = I = ACD$ ,  $AI = A = A^2CD = CD$ , and the complete system of confounding is as follows:

$$\begin{array}{ll}
 D = AC & C = AD \\
 I = ACD & AB = BCD \\
 A = CD & BC = ABD \\
 B = ABCD & BD = ABC
 \end{array} \quad (160)$$

Defining Contrasts and the Principal Block. - The next step in designing fractional factorial experiments by group theory methods is to determine which tests must be made to obtain the desired confounding of coefficients. This is automatic in the method of confounding by selecting tests from a table of signs for two-level factorial designs. However, when using group theory methods, it is necessary to make use of the concepts of defining contrasts and the principal block.

In any system of confounding, the set of defining contrasts is the set of aliases which contains the coefficient I. This set is so named because it serves to define the complete system of confounding, and it is used also to determine the tests which are to be made. The complete system of confounding is defined by the set of defining contrasts, because this set of aliases and group multiplication are used to find all other sets of aliases. The tests to be made are selected by first using the defining contrasts to find the tests in the principal block. Then the principal block and a group multiplication operation defined for test symbols are used to find the tests in other blocks. Finally, one of the blocks of tests is selected for an experiment.

The principal block of tests is the fractional replicate design which contains the test (1); that is, the test in which all factors are at their lowest level. The group theory procedures require that this set of tests be found first; then the other possible sets of tests are found by using the principal block and the group multiplication operation. The tests in the principal block are found by expressing both tests and defining contrasts in expanded notations.

For example, in the roasting experiment with the system of confounding given by the pairs of aliases in array (160), ACD is the coefficient of the interaction effect for the factors residence time, type of chemical analysis, and type of ore. The test ab is made at the higher levels of residence time and roasting temperature and the lower levels of type of analysis and type of ore. The coefficient ACD also is written  $A^1 B^0 C^1 D^1$ , and the test ab also is written  $a_1 b_1 c_0 d_0$ . Each coefficient can be written in the form  $A^p B^q C^r D^t$ , and each test can be written in the form  $a_v b_w c_x d_y$  where, in this example, p, q, r, t, v, w, x, and y can equal zero or 1. In the expanded notation, the test  $a_v b_w c_x d_y$  is compared with the coefficient  $A^p B^q C^r D^t$  by obtaining the sum  $p_v + q_w + r_x + t_y$ . For the test ab and the coefficient ACD, the corresponding sum  $(1)(1) + (0)(1) + (1)(0) + (1)(0) = 1$ . On the other hand, for the test ac and the coefficient ACD, the sum is  $1 + 0 + 1 + 0 = 2$ . The rule for finding the tests in the principal block is expressed as follows:

A test is in the principal block if the comparison between that test and each of the defining contrasts gives a sum equal to zero or a multiple of 2; that is, if,

$$p_v + q_w + r_x + t_y = 2n, n = 0, 1, 2, \dots \quad (161)$$

The comparison between any test and the coefficient I gives the sum  $0 + 0 + 0 + 0 = 0$ . Therefore, the essential comparisons are those between each of the tests and all other coefficients in the set of defining contrasts.

In the roasting experiment, the defining contrasts are I and ACD, and so each test must be compared with coefficient ACD. In this case,  $p = 1$ ,  $q = 0$ ,  $r = 1$ , and  $t = 1$ . These comparisons are shown as follows:

Test symbol	pv	qw	mx	ty	Sum
(1)	0	0	0	0	0
a	1	0	0	0	1
b	0	0	0	0	0
c	0	0	1	0	1
d	0	0	0	1	1
ab	1	0	0	0	1
ac	1	0	1	0	2
ad	1	0	0	1	2
bc	0	0	1	0	1
bd	0	0	0	1	1
cd	0	0	1	1	2
abc	1	0	1	0	2
abd	1	0	0	1	2
acd	1	0	1	1	3
bcd	0	0	1	1	2
abcd	1	0	1	1	3

The tests in the principal block are those for which the sum is zero or 2; that is,

$$(1), b, ac, ad, cd, abc, abd, \text{ and } bcd. \quad (162)$$

The other block consists of the remaining tests; that is,

$$a, c, d, ab, bc, bd, acd, \text{ and } abcd. \quad (163)$$

Either of the two blocks of tests (162) or (163) can be used to obtain the system of confounding given by the pairs of aliases in array (160).

In a two-level experiment with any number of factors  $X_a, X_b, X_c, \dots, X_k$ , the tests in the principal block are found by calculating sums of products of corresponding superscripts and subscripts similar to the sum on the left side of equation (161). The test  $a_v b_w c_x \dots k_z$  is in the principal block if for each coefficient  $A^p B^q C^r \dots K^u$  in the set of defining contrasts, the sum

$$pv + qw + rx + \dots + uz = 2n, \quad n = 0, 1, 2, \dots \quad (164)$$

where  $p, q, r, \dots, u, v, w, x, \dots, z = 0$  or  $1$ . If a larger number of factors and, therefore, a larger number of tests are involved in an experiment, it is tedious to compare all tests with the coefficients in the set of defining contrasts. After some tests in the principal block have been found, the others can be found by a method now to be given.



The tests in the principal block together with the proper operation form a group. The operation is group multiplication defined for two-level factorial designs so that

$$a^2 = b^2 = c^2 = d^2 = \dots = 1. \quad (165)$$

A test symbol represents a particular combination of factor levels in an experiment and is not a number in the elementary algebraic sense. Therefore, the product of test symbols is purely a symbolic device used for finding the tests in a fractional factorial design. Expression (165) states that whenever a letter is squared in the product of tests in a two-level factorial design, the square is either omitted from the product or replaced by 1. With this definition, the product of any two tests in this group will be another test in the same group. For example, the tests  $ac$  and  $ad$  are in the principal block (162); the product  $(ac)(ad) = a^2cd = cd$  which also is in the principal block. To make use of this property in a systematic way, the tests may be compared as follows: Compare the tests represented by one letter in alphabetical order with the defining contrasts, then the tests represented by two letters also in alphabetical order, and so on until three tests, other than test (1), have been found. These three tests should be independent in the sense that the product of any two or all three of them is not one of these three tests. The first three tests in this example are  $b$ ,  $ac$ , and  $ad$ . These may be multiplied together in pairs to find three additional tests; that is,  $(b)(ac) = abc$ ,  $(b)(ad) = abd$ , and  $(ac)(ad) = cd$ . All three may be multiplied together to find another test,  $(b)(ac)(ad) = bcd$ . There must be eight tests in the half-replicate design, so as soon as eight tests have been found, the design is complete.

These eight tests, (1),  $b$ ,  $ac$ ,  $ad$ ,  $abc$ ,  $abd$ ,  $cd$ , and  $bcd$ , are the same as those previously found in the principal block (162). If there are 16 tests in the principal block of a fractional factorial design, it is necessary to find four independent tests in order to obtain enough products to find the remaining tests. If there are 32 tests, 5 independent tests must be found. In general, if there are  $2^n$  tests in the design,  $n$  independent tests must be found.

A relationship exists between the tests in the principal block and those in the other blocks for fractional factorial designs that is used when there are more than two blocks from which to choose. For example, in the case of a quarter-replicate design, there are four possible blocks, and the relationship is used to find the three nonprincipal blocks. This relationship uses the group multiplication operation defined by expression (165) for the test symbols in two-level factorial designs and can be explained by referring to the principal block (162). First, any test which is not in the principal block must be selected. One such test is the test  $a$ . Then each test in the principal block is multiplied by  $a$  to find the other tests in the second block. Thus  $a(1) = a$ ,  $a(b) = ab$ ,  $a(ac) = c$ , and so on. When the tests in block (162) are successively multiplied by  $a$ , the tests in block (163) are obtained in the following order:  $a$ ,  $ab$ ,  $c$ ,  $d$ ,  $acd$ ,  $bc$ ,  $bd$ , and  $abcd$ . Any of the other tests in block (163) could have been used with the tests in the principal block to find the remaining tests in block (163). In each case, the tests would be found in a different order.

If there are three nonprincipal blocks, as in the case of a quarter-replicate design, one test that is not in the principal block is selected, and with this test, the remaining tests in one nonprincipal block are found. Then another test that is in neither the principal block nor the first nonprincipal block is selected, and the tests in a second nonprincipal block are found. The tests which have not been found in the principal or first two nonprincipal blocks are in the third nonprincipal block.

It may be necessary to know not only that two coefficients are aliases, but also to know exactly how they are confounded in a particular design. For example, it is sometimes necessary to use a fractional factorial design even though two important effects are confounded with each other. In this case, it may be possible to use two or more different fractional factorial designs in order to obtain separate estimates of the two effects. This is discussed further in the next section on partial confounding. However, the following observation about the various blocks in two-level designs will be helpful in designing such experiments. If the response function were written out for each test in the principal block (162), it would be found that the data obtained could be used to calculate the sum of confounded coefficients  $I - (1/8)ACD$ . The procedures for this calculation are indicated in the set of equations (148) in the first section under fractional factorial designs and confounding. The data from the tests in the second block (163) can be used to calculate the sum  $I + (1/8)ACD$ . If a four-factor experiment is designed in which  $I$  is confounded with  $ABCD$ , the data from the corresponding principal block will yield  $I + (1/16)ABCD$ . Each coefficient in a sum of defining contrasts is multiplied by  $(1/2)^n$ , where  $n$  is the number of letters in the coefficient representing factors. The sign of each coefficient in the sum of defining contrasts for a principal block may be determined as follows: A coefficient is even if it contains letters corresponding to an even number of factors, and odd if it contains letters corresponding to an odd number of factors. In the sum of defining contrasts for the principal block, the even coefficients are positive and odd coefficients are negative. Coefficient  $I$  contains no letters corresponding to factors and is always even. Coefficient  $ACD$  is odd. Therefore, data from the principal block (162) will yield  $I - (1/8)ACD$ .

The signs of the coefficients in the sums of defining contrasts corresponding to the nonprincipal blocks are determined from the signs in the sum of defining contrasts for the principal block as follows: A test is selected in the block for which the signs are to be determined. In the roasting experiment, the test  $a$  is in the nonprincipal block (163). The coefficients in the sum corresponding to the principal block which contain the letter  $A$  are each multiplied by  $(-1)$ . The letter  $A$  in the coefficient symbol corresponds to the letter  $a$  in the test symbol. In this example, the result is  $I + (1/8)ACD$ , and this is the sum corresponding to block (163). Any other test in this block could have been used. Consider the test  $abcd$ . Each coefficient containing the letters  $A$ ,  $B$ ,  $C$ , or  $D$  is multiplied once by  $(-1)$  for each of these letters which it contains. If the coefficient contains two of these letters, it is multiplied by  $(-1)^2$ ; if it contains three of these letters, it is multiplied by  $(-1)^3$ , and so on. The coefficient  $ACD$ , therefore, is multiplied by  $(-1)^3$  and, again, we obtain  $I + (1/8)ACD$ . As another example,



consider a quarter-replicate design with the following set of defining contrasts: I, ACE, BDE, and ABCD. The principal block for this design will yield the sum

$$I - (1/8)ACE - (1/8)BDE + (1/16)ABCD. \quad (166)$$

One of the nonprincipal blocks contains the test be. Therefore, the sum corresponding to this block is

$$\begin{aligned} I - (-1)(1/8)ACE - (-1)^2(1/8)BDE + (-1)(1/16)ABCD \\ = I + (1/8)ACE - (1/8)BDE - (1/16)ABCD. \end{aligned} \quad (167)$$

It remains to determine how the other sets of aliases are confounded in any block. If the defining contrasts are confounded as shown in the sum (166), then the sum for the coefficient A and its aliases is found in the following way: Each coefficient in the sum (166) together with its sign is multiplied by A to obtain A, -CE, -ABDE, and BCD. Then each coefficient so obtained is multiplied by  $(1/2)^{n-1}$ , where n is the number of letters in the coefficient. Thus the sum so obtained is

$$A - (1/2)CE - (1/8)ABDE + (1/4)BCD. \quad (168)$$

In this example, similar sums can be obtained for the coefficients B, C, D, E, and their respective aliases. The sum for the coefficient AB and its aliases also is found by multiplying each coefficient in the sum (166) together with its sign by AB. In this case, each coefficient then is multiplied by  $(1/2)^{n-2}$ , since there are two letters in the coefficient AB, and the sum obtained is

$$AB - (1/2)BCE - (1/2)ADE + CD. \quad (169)$$

A similar sum can be obtained for the coefficient AD and its aliases. This procedure can be applied to any system of confounding.

Higher order effect coefficients also are confounded in a two-level factorial design. Ordinarily, the range of values for each factor will be selected so that such coefficients are not expected to be important. However, one should be aware of the manner in which higher order coefficients can influence the estimates of lower order coefficients. The definition of group multiplication for two-level designs states that the quadratic components of all main effects are confounded with the average effect coefficient I; that is,  $A^2 = B^2 = \dots = I$ . Cubic components of the main effects will be confounded with the corresponding linear components, for example,  $A^3 = AA^2 = AI = A$ . If higher order components of the interaction effect are important, their coefficients also will be confounded with lower order coefficients, namely,  $AB^2 = A$ ,  $A^2B = B$ ,  $A^2B^2 = I$ , and  $A^3B = AB^3 = A^3B^3 = AB$ . In general,  $A^pB^q$  will be confounded with I if both p and q are even, with A if p is odd and q is even, with B if p is even and q is odd, and with AB if both p and q are odd.

Partial Confounding. - Partial confounding is used in an experiment when it is necessary to make the tests in different blocks and yet all interactions



among the major factors are important. Two or more fractional factorial designs are included in such an experiment so that the block effects can be confounded with different interaction effects in each design. The interaction effects which are confounded with block effects in any particular fractional factorial design cannot be estimated by the tests in that design. Therefore, it is necessary to include additional fractional factorial designs so that each of the major factor interaction effects can be estimated by the tests in at least one of the designs.

Let a two-level factorial experiment be designed to study the effects upon metal extraction of time,  $X_a$ , temperature,  $X_b$ , and base concentration,  $X_c$ , during leaching of a calcine previously prepared under reducing conditions. The data from this experiment will be used to calculate the coefficients I, A, B, C, AB, AC, BC, and ABC, all of which are expected to be important. The size of equipment available necessitates making the eight tests in two blocks of four tests. The reduced calcine must not be exposed to the air, and it is, therefore, difficult to blend the calcines from several different roasts before leaching. It is possible to make only enough calcine for four leaches during a single roast. Minor variations in furnace conditions from one roast to another may affect the results obtained. As before, the effect of using calcines from different roasts is regarded as the effect of factor  $X_d$ , and interactions between factor  $X_d$  and the three principal factors, time, temperature, and concentration, are unimportant.

Two experiments can be designed so that calculations of all important coefficients can be obtained. One experiment can be designed in which coefficient D is confounded with coefficient ABC. If the principal block is used, the results of this experiment can be used to calculate I, A, B, C, AB, AC, BC, and the sum  $D + (1/4)ABC$ . Since both D and ABC are important, a second experiment must be designed in which D is confounded with another interaction coefficient, say AB. In this case, the nonprincipal block can be used, and the results of this second experiment can be used to calculate I, A, B, C, AC, BC, ABC, and the sum  $D + (1/2)AB$ . Now, the independent calculations of ABC from the data of the second experiment and AB from the data of the first experiment may be used to calculate D from the sums  $D + (1/4)ABC$  and  $D + (1/2)AB$ . By making the two experiments, the coefficients I, A, B, C, AC, and BC will be obtained with greater precision than AB and ABC, but all eight coefficients may be obtained in this way. If it should be desired to obtain all interaction coefficients with the same degree of precision, four experiments may be designed in which D is confounded with ABC in the first experiment, with AB in the second, with AC in the third, and with BC in the fourth. This method of designing two or more experiments to obtain calculations of important coefficients is called partial confounding.

#### Higher Degrees of Confounding for Two-Level Designs

Designs involving higher degrees of confounding are useful when testing several factors at two levels each and some or all of these factors do not interact, when it is necessary to introduce several minor factors into an experiment, and when tests are planned to select from several possible factors those which are more important for detailed investigation. The possibility of

using a relatively small fractional replicate design involving a higher degree of confounding deserves greater attention as the number of factors to be studied increases.

The procedure for designing fractional factorial experiments with higher degrees of confounding is an extension of the procedure already presented for half-replicate designs in the preceding sections. This procedure may be illustrated with the following example that involves the introduction of minor factors into an experiment. A vanadium ore is to be given a chloridizing roast to increase the vanadium extraction. Four factors are to be studied as follows: Temperature,  $X_a$ , at 750° and 800° C.; roasting time,  $X_b$ , at 1 and 2 hours; salt addition,  $X_c$ , at 6 and 9 percent of the charge; and particle size,  $X_d$ , at 1/4-inch and 10-mesh (0.065-inch). The full two-level factorial design for four factors requires 16 tests. There is room for four charges in the roasting furnace, and there is a possibility that eddy currents and other furnace characteristics may cause variations in roasting conditions in different locations in the furnace. The principles of confounding are used to select the location for each test charge so that effects due to differences in location will not be confounded with the more important major factor effects.

The four furnace locations can be regarded as four levels of a qualitative location factor,  $X_e$ . The effect of this factor can be analyzed for linear, quadratic, and cubic components with the coefficients  $E$ ,  $E^2$ , and  $E^3$ , respectively. However, since the present discussion is focused upon two-level designs, the coefficient  $E^2$  can be replaced with  $F$  and  $E^3$  with  $EF$ . The result will be a design based on the arbitrary assumption that there are two location factors,  $X_e$  and  $X_f$ . The interaction effect between  $X_e$  and  $X_f$  corresponds to the cubic component of the effect of a single location factor at four levels. The resulting design and subsequent evaluation of the effects of the major factors will be the same whether one location factor at four levels or two location factors each at two levels are assumed. The assumption of two factors is made in other literature<sup>10</sup> and permits the experiment to be designed as a two-level experiment. All interaction effects involving both major experiment factors and location factors are considered to be negligible.

The system of confounding that prevents location effects from being confounded with the more important major factor effects is obtained by designing a quarter replicate of a full six-factor, two-level factorial design. Each of the location effect coefficients  $E$ ,  $F$ , and  $EF$  is to be confounded with one of the major effect coefficients. In general, the coefficients of the higher order interaction effects of the major factors, that is, those interaction effects involving a larger number of factors, are confounded with the location effect coefficients. Some caution is necessary in selecting the coefficients to be confounded; for example, if  $E$  is confounded with  $ABCD$  and  $F$  with  $ABC$ , then  $EF$  will be confounded with the product  $(ABCD)(ABC)$ . The symbolic group theory notation for two-level designs given in expression (158) states that  $A^2 = B^2 = C^2 = D^2 = E^2 = F^2 = I$ . Therefore, any letter which is squared in a

<sup>10</sup>Davies, O. L., *Design and Analysis of Industrial Experiments*: Hafner Publishing Co., New York, N.Y., 2d ed., 1956, pp. 387-389.



product of coefficients is omitted, and  $(ABCD)(ABC) = D$ . Thus, EF is confounded with the main effect coefficient D. A more desirable selection is to let E be confounded with ABC and F with ABD. Then EF will be confounded with the product  $(ABC)(ABD) = CD$ . This latter selection is expressed in group theory notation as follows:

$$E = ABC, F = ABD, \text{ and } EF = CD. \quad (170)$$

The set of defining contrasts for the complete system of confounding is determined by the three pairs of aliases (170). The symbolic equality  $E = ABC$  is preserved if both sides are multiplied by E. Therefore,  $E^2 = ABCE$ , but  $E^2$  is confounded with I, and so  $I = ABCE$ . Similarly,  $F^2 = ABDF$  and  $E^2 F^2 = CDEF$  and the set of defining contrasts is

$$I, ABCE, ABDF, CDEF. \quad (171)$$

Now to find the aliases of coefficient A, each coefficient in the set of defining contrasts is multiplied by A to obtain  $AI = A$ ,  $A(ABCE) = BCE$ ,  $A(ABDF) = BDF$ , and  $A(CDEF) = ACDEF$ . The main and interaction effects of the four factors,  $X_a$ ,  $X_b$ ,  $X_c$ , and  $X_d$ , are of major importance, and the aliases of each corresponding coefficient are as follows:

A,	BCE,	BDF,	ACDEF;
B,	ACE,	ADF,	BCDEF;
C,	ABE,	ABCDF,	DEF;
D,	ABCDE,	ABF,	CEF;
AB,	CE,	DF,	ABCDEF;
AC,	BE,	BCDF,	ADEF;
AD,	BCDE,	BF,	ACEF;
BC,	AE,	ACDF,	BDEF;
BD,	ACDE,	AF,	BCEF;
CD,	ABDE,	ABCF,	EF;
ABC,	<u>E</u> ,	CDF,	ABDEF;
ABD,	CDE,	<u>F</u> ,	ABCEF;
ACD,	BDE,	BCF,	AEF;
BCD,	ADE,	ACF,	BEF;
ABCD,	DE,	CF,	ABEF.

Each of the major factor effect coefficients is confounded with three negligible coefficients of interaction effects involving both major factors and location factors with the exception of the three coefficients ABC, ABD, and CD. Therefore, a design with this system of confounding can be used to estimate the main effects and most of the interaction effects of the major factors without interference due to effects of different locations in the furnace.

The next step in designing a quarter-replicate design with the system of confounding given by the sets of aliases (171) and (172) is to determine the 16 tests which must be made. As explained in the section on defining contrasts and the principal block, each test in the full six-factor, two-level



factorial design must be compared in a systematic way with each coefficient in the set of defining contrasts (171) in order to find the tests in the principal block. In this case, each test must be compared with three coefficients, other than I, instead of one as in the case of half-replicate designs. The test  $a_u b_v c_w d_x e_y f_z$  is compared with the coefficient  $A^n B^p C^q D^r E^s F^t$  by obtaining the sum  $nu + pv + qw + rx + sy + tz$ . If a sum equal to zero or a multiple of 2 is obtained for a particular test and each of the defining contrasts, that test is in the principal block. There are  $16 = 2^4$  tests to be found, and so four independent tests must be found by direct comparison with the defining contrasts before the remaining tests can be found by group multiplication of the test symbols. The first four independent tests in the principal block are

$$ab, ce, df, acd. \quad (173)$$

These are multiplied together in pairs to obtain six additional tests:

$$abce, abdf, bcd, cdef, ade, acf. \quad (174)$$

The first four tests (173) are multiplied together in sets of three to obtain four more tests:

$$abcdef, bde, bcf, aef. \quad (175)$$

Finally, all four tests (173) are multiplied together to give

$$bef. \quad (176)$$

These 15 tests together with test (1) make up the principal block of the quarter-replicate design. The other three design blocks are found by the procedure discussed in the section on defining contrasts and the principal block. The letters e and f in the test symbols serve to identify the furnace location in which each of the 16 tests is to be made. The four test symbols in the principal design block that contain neither e nor f represent tests to be made in location 1 in the furnace. The symbols that contain e but not f represent tests to be made in location 2, those that contain f but not e represent tests to be made in location 3, and those that contain both e and f represent tests to be made in location 4. After the locations are identified, the letters e and f are omitted from all symbols and the 16 tests in the original four-factor experiment are divided among the four furnace locations as follows:

<u>Location</u>	<u>Tests</u>	
1	(1), ab, acd, bcd	
2	c, abc, ad, bd (e omitted)	(177)
3	d, abd, ac, bc (f omitted)	
4	cd, abcd, a, b (ef omitted)	

If one of the design blocks other than the principal block had been used, the 16 original tests would be divided among the four locations in the same way. For example, one design block contains the tests ef, abef, acdef, and bcdef, and 12 other tests. When the letters ef are omitted from these first

four symbols, the tests become (1), ab, acd, and bcd which are the same four tests assigned to location 1 in (177).

The 16 tests in the original four-factor experiment have been divided among four locations or four experiment blocks. The usual procedure now would be to make the tests in each block in a random order; that is, tests (1), ab, acd, and bcd would be made in a random order in one block of tests, then tests c, abc, ad, and bd in a random order in a second block of tests, and so on. In the present example, a block of tests represents four tests to be made in a particular furnace location, one test in each of four different furnace campaigns. The order in which the tests are made cannot be randomized in all locations because the four tests in any one furnace campaign must all be made at the same temperature. However, the tests can be assigned to furnace campaigns in the following way: Tests (1), c, d, and cd are to be made in locations 1, 2, 3, and 4, respectively, and are each to be made at 750° C. for 1 hour. These four tests are made during one campaign. Similarly, tests ab, abc, abd, and abcd at 800° C. for 2 hours are made during another campaign. Tests acd, ad, ac, and a at 800° C. for 1 hour are made during a third campaign, and tests bcd, bd, bc, and b at 750° C. for 2 hours are made during a fourth campaign. The four campaigns are conducted in a random order.

When an experiment involving higher degrees of confounding is to be designed, it is helpful to know that the set of defining contrasts is a subgroup. A subgroup is a set of some of the members of a known group that, together with the operation defined for the known group, also satisfies the requirements of a group. For example, the 64 coefficients in a six-factor, two-level factorial experiment and the group multiplication operation constitute a group. Of these 64 coefficients, the four in the set of defining contrasts (171), I, ABCE, ABDF, and CDEF, and group multiplication also constitute a group. The identity member is I, each coefficient is its own inverse, and the product of any two of these coefficients also is one of the defining contrasts, for example, (ABCE)(ABDF) = CDEF. The fact that the set of defining contrasts for any system of confounding is a subgroup makes it possible to find some of the coefficients in the set of defining contrasts by group multiplication of other coefficients known to be in the set.

The following example shows how a high degree of confounding can be used in the design of an experiment for preliminary research. Sometimes a research problem involves a large number of factors that may influence the response to be investigated. There is not enough time to investigate all factors thoroughly, so a selection of the more important factors must be made. A fractional factorial design with a high degree of confounding can be used as a guide in making the selection.

Consider the flotation of a beryllium mineral from a complex ore in which the following seven factors may influence the results. The first factor,  $X_a$ , is the addition of sodium fluoride to the slurry before conditioning at two levels, 2.25 and 4.25 pounds sodium fluoride per ton of solids. The second factor,  $X_b$ , is the time at which sodium fluoride is added to the slurry. The two levels of this factor are qualitative, and the sodium fluoride is to be added before or after grinding. The third factor,  $X_c$ , is the conditioning



time of the slurry after grinding and before other reagents are added to the slurry. The levels of  $X_c$  are 5 and 15 minutes. The fourth factor,  $X_d$ , is the addition of sodium hexametaphosphate to the slurry in the amounts of 2.25 and 2.75 pounds per ton of slurry. The fifth factor,  $X_e$ , is the conditioning time after the phosphate salt has been added and before the collector is added to the slurry. The levels of  $X_e$  are 5 and 10 minutes. The sixth factor,  $X_f$ , is the addition of collector to the slurry. The collector is a mixture of oleic acid and kerosene. The amount of oleic acid is constant at 1 pound per ton, but the amount of kerosene is to be studied at two levels, 0.5 and 1 pound per ton of solids. The seventh factor,  $X_g$ , is the final conditioning time after the collector has been added and the levels are 5 and 10 minutes.

A fractional factorial design for this experiment will reduce the number of tests needed for a preliminary evaluation of the seven factors. A full two-level factorial design for seven factors requires 128 tests, and if some tests are to be duplicated to obtain an estimate of experimental error, the number of tests is larger than 128. A one-sixteenth replicate of this design contains eight tests and can be designed so that no two main effect coefficients are confounded with each other. Each coefficient will be confounded with 15 other aliases, so there is a chance of some bias in the estimates of the main effect coefficients. However, the results of the experiment can be used as a guide to select the factors which are more important for more thorough investigation.

Previous experience with the factors under investigation can be used in designing the fractional factorial experiment so as to minimize the chance of bias in the main effect estimates. The response surface upon which statistical evaluation of the data is based can be approximated over a sufficiently small region by a plane surface which represents only linear main effects of each of the factors. Within this small region, interaction effects are less important than they are over larger regions. Now, consider factor  $X_a$  in the flotation experiment. The practical range of levels for this factor may be, say, 0 to 10 pounds sodium fluoride per ton of solids. Previous experience shows that a difference of at least 2 pounds in the levels of this factor is necessary before a significant difference in the response values for two different tests can be obtained. Therefore, the levels in a two-level design should be 2 pounds apart. A larger spacing increases the chance for bias in main effect estimates because of interaction effects. Similar experience should guide the spacing of levels for each of the other factors. If previous experience is not available, then a reasonably small fraction of the practical range of levels should be used in preliminary research.

The one-sixteenth replicate of a seven-factor, two-level factorial experiment is designed as follows: Each main effect coefficient is confounded with 3 two-factor interaction effect coefficients and 12 higher order coefficients by confounding A with BE, CF, and DG in one set of aliases and B with DF in another set; that is,

$$A = BE = CF = DG, \text{ and } B = DF.$$

(178)



Four coefficients in the set of defining contrasts are determined by the aliases in set (178). These are

$$ABE, ACF, ADG, BDF. \quad (179)$$

The remaining 11 coefficients in the set are found by making use of the fact that the coefficients in the set of defining contrasts and group multiplication constitute a subgroup. Since this is true, the remaining 11 coefficients can be found as products of the 4 coefficients in set (179). Six coefficients are obtained as products of pairs of the coefficients in set (179):

$$BCEF, BDEG, ADEF, CDFG, ABCD, ABFG. \quad (180)$$

Four more are found as products of three of the coefficients in set (179):

$$ABCDEFG, CDE, EFG, BCG. \quad (181)$$

The last coefficient is obtained as the product of all four coefficients in set (179).

$$ACEG. \quad (182)$$

The 15 coefficients in sets (179), (180), (181), and (182) and the coefficient I are the coefficients in the set of defining contrasts for a one-sixteenth replicate design.

There are eight tests in the principal block for this design, and three independent tests are found by comparison of the tests in the seven-factor, two-level design with each of the 15 coefficients in sets (179), (180), (181), and (182). The remaining four tests are found as products of the three independent tests, and the tests in the principal block are

$$(1), abcd, abfg, aceg, cdfg, bdeg, bcef, adef. \quad (183)$$

There are 15 other blocks of eight tests that may be obtained, and any one of these or the principal block (183) may be used to obtain estimates of the main effect coefficients A, B, C, D, E, F, and G, as well as the average effect coefficient I. If there were no other estimate of experimental error available, the eight tests in the block being selected should be duplicated to obtain an experimental error estimate for comparison with each of the main effect estimates.

The experiment based upon the one-sixteenth replicate design in the preceding discussion is the first step in the investigation of the seven factors. The next step is determined by the results of the first experiment. One possible result is for the main effect estimates of three of the factors to be significantly greater than the other four main effect estimates. Suppose the three factors are  $X_d$ , addition of sodium hexametaphosphate to the slurry;  $X_e$ , the conditioning time after the phosphate salt has been added; and  $X_g$ , the final conditioning time after collector has been added. Then subsequent experiments would be planned to investigate the main and interaction effects of

these three factors in greater detail. For the subsequent tests the other four factors would be held at constant levels.

Another possible result of the data obtained from the one-sixteenth replicate experiment is for all main effect estimates to be sufficiently large to require further investigation before any of the factors are eliminated. In this case, the design can be expanded to a one-eighth replicate design by making eight additional tests. These eight tests can be determined by the following considerations: It generally is assumed that higher order interaction effects will be less significant than those of lower order. Therefore, the next step will be to design the experiment so as to separate main effect coefficients from two-factor interaction effect coefficients. The procedures used here were introduced in the section on defining contrasts and the principal block. Suppose the principal block of tests (183) had been made in the first experiment. The responses from these eight tests can be combined algebraically to obtain eight sums of aliases. One of these will be the sum of defining contrasts in which even coefficients are positive and odd coefficients are negative; that is,

$$\begin{aligned} I &= (1/8)ABE - (1/8)ACF - (1/8)ADG - (1/8)BDF + (1/16)BCEF \\ &+ (1/16)BDEG + (1/16)ADEF + (1/16)CDFG + (1/16)ABCD \\ &+ (1/16)ABFG - (1/128)ABCDEFG - (1/8)CDE - (1/8)EFG \\ &- (1/8)BCG + (1/16)ACEG. \end{aligned} \quad (184)$$

From this sum (184) the sums containing each of the main effect coefficients can be obtained; for example, the sum containing the coefficient A is

$$\begin{aligned} A &= (1/2)BE - (1/2)CF - (1/2)DG - (1/8)ABDF + (1/16)ABCEF \\ &+ (1/16)ABDEG + (1/4)DEF + (1/16)ACDFG + (1/4)BCD + (1/4)BFG \\ &- (1/32)BCDEFG - (1/8)ACDE - (1/8)AEFG - (1/8)ABCG + (1/4)CEG. \end{aligned} \quad (185)$$

For the present discussion, attention is focused upon main effects and two-factor interaction effects such as the first four terms in sum (185); that is,  $A - (1/2)BE - (1/2)CF - (1/2)DG$ . The eight additional tests to be made must constitute a one-sixteenth replicate experiment which will yield a sum whose first four terms are  $A + (1/2)BE + (1/2)CF + (1/2)DG$ . These tests are found by finding the nonprincipal block with the sum of defining contrasts similar to the sum (184) but in which all terms are positive. The block containing the test *abe* yields the desired sum. Each term in sum (184) which contains one of the letters A, B, or E is multiplied by  $(-1)$ ; each term containing two of the letters is multiplied by  $(-1)^2$ ; and each term containing all three letters is multiplied by  $(-1)^3$ . The other tests are found by multiplying each test in the principal block (183) by *abe*. The eight additional tests are

$$abe, cde, efg, bcg, abcdefg, adg, acf, bdf. \quad (186)$$

The expanded design consisting of the tests in the principal block (183) and the block (186) constitutes the principal block of a one-eighth replicate design in which all main effect coefficients are separated from two-, four-,



and six-factor interaction effect coefficients. Main effects still will be confounded with three- and five-factor interaction effects. The assumption that higher order interaction effects are less significant than lower order interaction effects means that the main effect estimates obtained from the one-eighth replicate design can be compared and the more important factors selected with greater confidence. At this point, the more important factors may be studied in greater detail, or the one-eighth replicate design can be expanded to a one-quarter replicate design by making 16 additional tests.

Other blocks than the principal blocks of the one-sixteenth replicate design can be expanded to separate main effect coefficients from two-factor interaction effect coefficients. For example, one block contains the test a. The other tests in this block are found by multiplying each of the tests in the principal block (183) by letter a to obtain

a, bcd, bfg, ceg, acdfg, abdeg, abcef, def. (187)

The eight additional tests to expand this block to a one-eighth replicate design are found by multiplying each of the tests (186) also by letter a to obtain

be, acde, aefg, abcg, bcdefg, dg, cf, abdf. (188)

The results of the 16 tests in sets (187) and (188) will yield estimates of the main effects separated from the two-factor interaction effects.

In the case of factors which do not interact with each other, a fractional factorial design with a high degree of confounding can be used directly to obtain estimates of the main effects. It may be desired to evaluate the effects of several qualitative or minor factors upon a given response. Such factors include the performance of different men or different machines, the making of tests on different days, and so on. When several such factors are to be tested, the smallest fractional factorial design which gives separate estimates of all main effects is used.

#### Confounding in Factorial Designs Having More Than Two Levels per Factor

As more levels per factor are included in a design, a more complete evaluation of the effects of the factors can be made over a given range of values for each factor. If some of the higher order components of the effects are not important, it is still desirable to estimate the lower order components over a larger number of levels per factor. In this case a full factorial design may require more tests and give more information than necessary. The general procedure for confounding, which has been introduced in terms of the simpler two-level designs, can be extended for the design of experiments having more than two levels per factor so as to reduce the number of tests and yet permit the evaluation of the important effects over the desired number of levels. The general procedure has the advantage that it can be used in more extensive designs, whereas the method based upon a table of signs cannot.



An example in which the principles of confounding are useful in a design involving more than two levels per factor is the following: There are three factors to be studied, each at four levels. In this case, a full factorial design requires 64 tests. An experiment based upon this design will yield data from which to calculate the coefficients  $I, A, A^2, A^3, B, B^2, B^3, C, C^2, C^3$ , and 54 interaction coefficients. It may be known that only linear and quadratic components of the main effects and the lower order components of the two-factor interaction effects are important. A one-fourth replicate of the full four-level design contains 16 tests and can be used to calculate  $I, A, A^2, B, B^2, C, C^2, AB, AB^2, A^2B, AC, AC^2, A^2C, BC, BC^2$ , and  $B^2C$ . The set of defining contrasts for the design contains the aliases  $I, ABC, A^2B^2C^2$ , and  $A^3B^3C^3$ . For comparison, a full three-factor, three-level factorial design requires 27 tests, or 11 more tests than are necessary if the coefficients  $A^2B^2, A^2C^2, B^2C^2$ , and the various components of the three-factor interaction effect are not important. The one-fourth replicate of the four-level design also has the advantage of including four levels for each factor in the investigation. As the number of levels per factor increases, the possibility of reducing the number of tests by means of a fractional replicate of a full design deserves increasing attention.

The general procedure for confounding effects in fractional factorial designs now will be applied to designs in which each factor is studied at three levels. Three-level factorial experiments are designed to estimate linear and quadratic components of the main effect of each factor and the corresponding components of the interaction effects. Such designs cannot be used to estimate cubic components of the main effects. The general procedure for confounding in three-level designs is based upon the fact that coefficients of cubic components of main effects are confounded with the average effect coefficient  $I$ . This is expressed in group theory notation as follows:

$$A^3 = B^3 = C^3 = D^3 = \dots = I. \quad (189)$$

This corresponds to the similar expression (158) for two-level designs in which quadratic component coefficients  $A^2, B^2$ , and so forth are confounded with  $I$ . The coefficients for which a three-level factorial experiment is designed are multiplied together in the procedure for confounding effects.

Because of the relationship (189), the symbolic product of any set of the coefficients which are estimated by a three-level factorial experiment also will be one of these coefficients. For example,  $(A^2BC)(AB) = A^3B^2C$ , but  $A^3$  is confounded with  $I$  which serves as the identity and is omitted from any product unless it stands alone. Therefore,  $(A^2BC)(AB) = B^2C$ . Another example product is the following:  $(AB^2C)(B^2C^2) = AB^3BC^2 = AB$ . The set of coefficients for a three-level factorial design and group multiplication satisfies the mathematical requirements for a group. Products are members of the set, the identity member is  $I$ , and the inverse of each member is the square of that member; for example,  $(A)(A^2) = A^3 = I$ ; also  $(AB^2C)^2 = A^2B^4C^2 = A^2BC^2$ , since  $B^4 = B^3B = IB = B$ , and  $(AB^2C)(A^2BC^2) = I^3 = I$ .

Confounding in three-level designs will be illustrated by means of an experiment to study three factors,  $X_a, X_b$ , and  $X_c$ . The least number of

coefficients in a subgroup, and therefore in a set of defining contrasts, for a three-level design is three. One may choose  $I$  and any other coefficient, say  $A^2B$ , to be in the subset. The third member is the inverse of the second coefficient; in this case,  $(A^2B)^2 = AB^2$ . There are 13 possible subgroups in this example which contain three coefficients, and each of the 27 coefficients,  $I, A, A^2, \dots, A^2B^2C^2$ , will be in one of these subgroups. These 13 subgroups are shown in table 7 together with conventional symbols, which have been adopted in the literature<sup>11</sup> for more convenient reference to the subgroups in subsequent discussion.

TABLE 7. - The 13 subgroups of three coefficients which may be obtained from the group of 27 coefficients calculated from the data of a full three-factor, three-level factorial design

Subgroup	Corresponding symbol	Subgroup	Corresponding symbol
$I, A, A^2$	<u>A</u>	$I, B^2C, BC^2$	$I(BC)$
$I, B, B^2$	<u>B</u>	$I, BC, B^2C^2$	$J(BC)$
$I, C, C^2$	<u>C</u>	$I, A^2BC, AB^2C^2$	$W(ABC)$
$I, A^2B, AB^2$	$I(AB)$	$I, AB^2C, A^2BC^2$	$X(ABC)$
$I, AB, A^2B^2$	$J(AB)$	$I, ABC^2, A^2B^2C$	$Y(ABC)$
$I, A^2C, AC^2$	$I(AC)$	$I, ABC, A^2B^2C^2$	$Z(ABC)$
$I, AC, A^2C^2$	$J(AC)$		

A three-member set of defining contrasts may be used to design a one-third replicate of a full three-level design. The most useful of the subgroups in table 7 to be selected as defining contrasts are  $W(ABC)$ ,  $X(ABC)$ , and  $Y(ABC)$ . The data from an experiment based on one of these subgroups can be used to calculate both linear and quadratic component coefficients of all three factors and two of the three lowest order two-factor interaction component coefficients; that is,  $I, A, A^2, B, B^2, C, C^2$ , and two of the three coefficients  $AB, AC$ , and  $BC$ . Such an experiment consists of 9 tests, whereas the full three-level design consists of 27 tests.

The other subgroups in table 7 generally are less useful but may be of value in particular applications. The subgroup  $Z(ABC)$  may be used to calculate all main effect coefficients, but the lowest order interaction coefficients  $AB, AC$ , and  $BC$  are confounded with  $C^2, B^2$ , and  $A^2$ , respectively. The subgroup  $J(AB)$  confounds  $B^2$  with  $A$  and  $A^2$  with  $B$ ; therefore, this subgroup would be used only if  $A^2$  and  $B^2$  were known to be negligible, and it were desired to evaluate  $A$  and  $B$  over three levels for each corresponding factor. Both  $C$  and  $C^2$  can be obtained, and two components of each of the interaction effects between  $X_a$  and  $X_c$  and between  $X_b$  and  $X_c$  can be estimated; that is,  $AC, AC^2, BC$ , and  $BC^2$  can be calculated. Similar results are obtained with subgroups  $J(AC)$  and  $J(BC)$ . The subgroups  $I(AB), I(AC), I(BC), \underline{A}, \underline{B}$ , and  $\underline{C}$  cause some main effect coefficients to be confounded either with each other or with the average effect coefficient  $I$  and are of little value in designing fractional factorial experiments.

<sup>11</sup> Davies, O. L., Design and Analysis of Industrial Experiments: Hafner Publishing Co., New York, N.Y., 1956, p. 426.



The following example illustrates the use of one of the subgroups  $W(ABC)$ ,  $X(ABC)$ , or  $Y(ABC)$  to design a one-third replicate of a three-factor, three-level factorial experiment. Two factors are to be studied in a filtration experiment to estimate their effects upon the time required to filter a unit weight of a flotation concentrate. Factor  $X_a$  is the amount of flocculant added, and the levels are 0, 0.5, 1.0 pound per ton of concentrate. Factor  $X_b$  is the type of filter cloth used, and three types are included in the investigation. In addition, it is desired to compare the performances of three men who are being trained to make the tests for a more extensive investigation. The men are regarded as three levels of a personnel factor,  $X_c$ . The only interaction effect expected to exist is that between factors  $X_a$  and  $X_b$ , and only the lowest order component coefficient,  $AB$ , is expected to be important. A system of confounding based upon subgroup  $W(ABC)$  has the interaction effects coefficient  $BC$  confounded with the main effect coefficient  $A$ . Otherwise, the main effect coefficients and the two interaction coefficients  $AB$  and  $AC$  are confounded only with unimportant higher order interaction effect coefficients. A system of confounding based upon subgroup  $X(ABC)$  has  $AC$  confounded with  $B$ , and a system based upon subgroup  $Y(ABC)$  has  $AB$  confounded with  $C$ . In the present example,  $AB$  must not be confounded with a main effect coefficient. Therefore, either subgroup  $W(ABC)$  or  $X(ABC)$  may be selected for the design of a one-third replicate experiment. The subgroup  $X(ABC)$  is selected for this example.

The system of confounding for this experiment is determined in a way similar to that for two-level factorial designs. Each coefficient in the set of defining contrasts is multiplied by  $A$ , then by  $B$ , and so on, until all 27 coefficients have been located in a set of three aliases. With subgroup  $X(ABC)$  as the set of defining contrasts, the complete system of confounding is as follows:

$I,$	$AB^2C,$	$A^2BC^2;$	
$A,$	$A^2B^2C,$	$BC^2;$	
$B,$	$AC,$	$A^2B^2C^2;$	
$C,$	$AB^2C^2,$	$A^2B;$	
$A^2,$	$B^2C,$	$ABC^2;$	
$B^2,$	$ABC,$	$A^2C^2;$	
$C^2,$	$AB^2,$	$A^2BC;$	
$AB,$	$A^2C,$	$B^2C^2;$	
$BC,$	$AC^2,$	$A^2B^2.$	(190)

The tests in the principal block for this system of confounding are found by comparison with the defining contrasts. For three-level designs, test  $a_v b_w c_x \dots k_z$  is in the principal block if the comparison between that test and each of the defining contrasts  $A^p B^q C^r \dots K^u$  gives a sum equal to zero or a multiple of 3; that is,

$$pv + qw + rx + \dots + uz = 3n, \quad n = 0, 1, 2, \dots \quad (191)$$



Here,  $p, q, r, \dots, u, v, w, x, \dots, z$  can equal 0, 1, or 2. As in the case of two-level factorial designs, the tests in a full three-factor, three-level design are compared with the defining contrasts in alphabetical order, taking tests represented by one letter first, two letters second, and so on. Two independent tests in the principal block are

$$a_1 b_1, \quad a_2 c_1. \quad (192)$$

The remaining six tests, other than (1), can be found as indicated above, or the two tests (192) can be used as follows to find them:

When multiplying test symbols for designs having three or more levels, the subscripts are treated as powers; for example,  $(a)_1(a_1) = (a^1)(a^1) = a^2 = a_2$ . Group theory multiplication of test symbols in three-level factorial designs is defined so that

$$a_3 = b_3 = c_3 = d_3 = \dots = 1. \quad (193)$$

As a second example,

$$(a_2 c_1)(a_2 b_2) = a_4 b_2 c_1 = a_3 a_1 b_2 c_1 = a_1 b_2 c_1.$$

The remaining six tests in the principal block for the present example are found by taking all possible products of the two tests (192) and their squares; that is,

$$\begin{aligned} (a_1 b_1)^2 &= a_2 b_2, \\ (a_2 c_1)^2 &= a_1 c_2, \\ (a_1 b_1)(a_2 c_1) &= b_1 c_1, \\ (a_1 b_1)^2(a_2 c_1) &= a_1 b_2 c_1, \\ (a_1 b_1)(a_2 c_1)^2 &= a_2 b_1 c_2, \\ (a_1 b_1)^2(a_2 c_1)^2 &= b_2 c_2. \end{aligned} \quad (194)$$

Therefore, the nine tests in the principal block for a one-third replicate of a full three-factor, three-level, factorial design based upon the subgroup  $X(ABC)$  are

$$(1), a_1 b_1, a_2 c_1, a_2 b_2, a_1 c_2, b_1 c_1, b_2 c_2, a_1 b_2 c_1, \text{ and } a_2 b_1 c_2. \quad (195)$$

The other two design blocks for the same system of confounding are found by multiplying the tests in the principal block (195) by  $a_1$ , and then by  $b_1$  to obtain

$$a_1, a_2 b_1, c_1, b_2, a_2 c_2, a_1 b_1 c_1, a_1 b_2 c_2, a_2 b_2 c_1, b_1 c_2 \quad (196)$$

and

$$b_1, a_1 b_2, a_2 b_1 c_1, a_2, a_1 b_1 c_2, b_2 c_1, c_2, a_1 c_1, a_2 b_2 c_2. \quad (197)$$

The usefulness of the above procedure in finding the tests in the principal and other design blocks is the reason for the notation which has been adopted

for the tests in a factorial design; that is,  $a_{i-1}$  corresponding to response  $y_i$ , test  $a_{i-1}b_{j-1}c_{k-1}$  corresponding to response  $y_{ijk}$ , and test (1) corresponding to response  $y_{111}$ .

The tests in any one of the blocks (195), (196), or (197) can be made to obtain data from which to calculate the coefficients of the linear and quadratic components of the main effects of all three factors and the two interaction coefficients AB and BC, provided all other interaction coefficients are negligible. In the case where some of the other coefficients are not negligible, it is not possible, as it was with two-level experiments, to calculate algebraic sums for each set of aliases shown in the set (190) which are applicable to all responses obtained in the experiment. The reason for this is: The response function for the three-factor, three-level experiment under consideration is

$$\begin{aligned}\bar{y}_{ijk} = & IZ_{000}(ijk) + AZ_{100}(ijk) + A^2Z_{200}(ijk) + BZ_{010}(ijk) \\ & + \dots + AB^2CZ_{121}(ijk) + \dots + A^2BC^2Z_{212}(ijk) \\ & + \dots + A^2B^2C^2Z_{222}(ijk).\end{aligned}\quad (198)$$

In the system of confounding for the present example, the coefficients I,  $AB^2C$ , and  $A^2BC^2$  constitute one set of aliases. For any given response  $\bar{y}_{ijk}$ , the effects in equation (198) corresponding to these aliases are confounded and may be grouped as follows:

$$IZ_{000}(ijk) + AB^2CZ_{121}(ijk) + A^2BC^2Z_{212}(ijk). \quad (199)$$

The Z polynomials in equations (198) and (199) for a three-level experiment vary for the same response and also vary from response to response in absolute magnitude as well as in sign. Consequently, similar sums of the same components such as the sum (199) do not have a common absolute polynomial value which can be factored out of the sums for all responses, leaving a sum of aliases common to each response.

A one-third replicate of a three-level experiment may be designed by selecting any two coefficients to be confounded, instead of selecting one of the subgroups in table 7 as has been illustrated in the filtration experiment. One may know that a particular interaction coefficient is negligible and wish to confound it with one of the main effect coefficients. Suppose it is desirable to confound  $C^2$  with  $AB^2C$ . The defining contrasts then are found by multiplying each of these coefficients by C; that is,  $C^3 = AB^2C^2$  or  $I = AB^2C^2$ . The third defining contrast is  $(AB^2C^2)^2 = A^2BC$ . This set is the subgroup W(ABC). From here, the complete system of confounding and the tests in each block are found as shown in the last example. If two coefficients are selected as aliases, the system of confounding should be completed to determine whether any important coefficients are aliases of each other as a result of the initial selection.

Higher degrees of confounding can be used in three-level designs as well as in two-level designs. In such cases it usually is necessary that a larger number of factors be involved and that only main effects of the factors be

important. The coefficients in a three-level design can be listed in subgroups in which the number of coefficients is a power of 3; that is, 3, 9, 27, and so on. Any one of these subgroups may be selected as the set of defining contrasts from which to complete a system of confounding and find the tests in the principal and other design blocks.

The principles of confounding are readily extended to factorial designs having any number of levels per factor. If each factor were studied at four levels, the group multiplication would be defined so that

$$A^4 = B^4 = C^4 = \dots = I. \quad (200)$$

Any coefficient in a full four-level design can be placed in a subgroup in which the number of coefficients is a power of 4; that is, 4, 16, 64, etc. There are additional subgroups in the case of four-level designs in which some but not all of the coefficients can be placed; for example, there are some subgroups containing two coefficients. One coefficient is the average effect coefficient I, which serves as the identity element and must be in all subgroups. If there are three factors to be studied, the other coefficient in a subgroup containing two coefficients can be one of the following:

$$A^2, B^2, C^2, A^2B^2, A^2C^2, B^2C^2, \text{ or } A^2B^2C^2. \quad (201)$$

Additional special subgroups can be found in which the number of coefficients is a power of 2, other than those already mentioned in which the number is a power of 4. For example, the coefficients of set (201) together with I constitute a subgroup of eight coefficients. Any subgroup can be selected as a set of defining contrasts. A test  $a_v b_w c_x \dots k_z$  is in the principal block if the comparison between that test and each of the defining contrasts  $A^p B^q C^r \dots K^u$  gives a sum equal to

$$pv + qw + rx + \dots + uz = 4n, \quad n = 0, 1, 2, \dots, \quad (202)$$

where p, q, r, ..., u, v, w, x, ..., z can equal 0, 1, 2, or 3. Again,  $a_p$  is regarded as  $a^p$  and

$$a_4 = b_4 = c_4 = d_4 = \dots = 1. \quad (203)$$

With these relationships, the tests in the principal and other design blocks may be found.

In general, if each factor is studied at m levels, the group multiplication is defined so that

$$A^m = B^m = C^m = D^m = \dots = I. \quad (204)$$

Any coefficient in a full m-level design can be placed in a subgroup in which the number of coefficients is a power of m, that is, m,  $m^2$ ,  $m^3$ , and so on. In certain cases, a subgroup may contain some other number of coefficients. For example, if  $m = 6$ , the two coefficients I and  $A^3B^3$  form a subgroup, and also



the three coefficients  $I$ ,  $A^2B^4C^2$ , and  $A^4B^2C^4$  form a subgroup. A test is in the principal block if the appropriate sums are equal to

$$pv + qw + rx + \dots + uz = mn, \quad n = 0, 1, 2, \dots, \quad (205)$$

where  $p, q, r, \dots, u, v, w, x, \dots, z$  can equal  $0, 1, 2, \dots, (m - 1)$ . Finally,

$$a_m = b_m = c_m = d_m = \dots = 1. \quad (206)$$

These relationships may be used to design any fractional factorial experiment in which each factor is studied at  $m$  levels.

It also is possible to apply the principles of confounding to designs in which the factors are not all studied at the same number of levels. Confounding in such designs is complicated, the usefulness is limited, and Davies<sup>12</sup> recommends that it be avoided if possible. Additional information on confounding may be found in the book by Davies.

As in two-level designs, estimates of coefficients for an  $m$ -level design will be biased if main effect coefficients of order  $m$  or larger and corresponding interaction effect coefficients are important. If such a higher order coefficient,  $A^pB^qC^r \dots K^u$ , is important, the lower order alias may be determined by dividing each power,  $p, q, r, \dots, u$ , by  $m$ . The remainders obtained will be the respective powers of  $A, B, C, \dots, K$  in the alias.

Latin Squares. - There is frequent reference in the literature to Latin squares. A Latin square is simply one type of fractional factorial design and is used to study three factors which usually are qualitative and do not interact. If three levels are studied for each factor, the Latin square is a one-third replicate of a full three-factor design; if four levels, then it is a one-fourth replicate; if five levels, a one-fifth replicate; and so forth.

The construction of a Latin square gives a simple method for finding the tests in the corresponding full factorial design which are to be made. However, this procedure does not tell how the effects are confounded, and therefore, it should be used only when interactions between the factors are known to be nonexistent or negligible.

The following example illustrates the type of experiment that may employ a Latin square design. A preliminary investigation of manganese flotation is to be made. One purpose of this investigation is to determine whether to deslime the ore before flotation. Factor  $X_a$  is the type of ore, and the three levels studied are undeslimed ore and the two fractions, sands and slimes. Factor  $X_b$  is the type of flotation cell to use, and three levels to be studied are Denver, Fagergren, and Booth cells. Factor  $X_c$  is a personnel factor. This experiment is the first step in a more extensive investigation of manganese flotation, and three men are being trained to make the tests. Therefore,

<sup>12</sup>Davies, O. L., Design and Analysis of Industrial Experiments: Hafner Publishing Co., New York, N.Y., 1956, pp. 367-494.

an additional purpose of this experiment is to compare the performance of the three men. Interactions among these factors are not expected to be important, so a Latin square design can be used to reduce the number of tests required from 27 tests for a full factorial design to 9 tests. A Latin square design may include the following nine tests:

$$\begin{array}{ccc}
 (1) & b_1 c_1 & b_2 c_2 \\
 a_1 c_2 & a_1 b_1 & a_1 b_2 c_1 \\
 a_2 c_1 & a_2 b_1 c_2 & a_2 b_2
 \end{array} \quad (207)$$

This arrangement is obtained by first listing the tests in a full design for the two factors  $X_a$  and  $X_b$  in such a way that the rows represent the first, second, and third levels of factor  $X_a$  and the columns represent the first, second, and third levels of factor  $X_b$ . Then the letter  $c$  is added to the test symbols in such a way that each subscript appears once in each row and in each column. By rearranging the order of the subscripts of the letter  $c$  in the rows and columns, 11 other Latin square designs are possible for this particular experiment.

The characteristic property of the Latin square is more apparent if we list just the subscripts of the letter  $c$  in the same array:

$$\begin{array}{ccc}
 0 & 1 & 2 \\
 2 & 0 & 1 \\
 1 & 2 & 0
 \end{array} \quad (208)$$

Another possible arrangement of the subscripts is

$$\begin{array}{ccc}
 0 & 1 & 2 \\
 1 & 2 & 0 \\
 2 & 0 & 1
 \end{array} \quad (209)$$

This corresponds to a Latin square design for the same experiment which includes the following tests:

$$\begin{array}{ccc}
 (1) & b_1 c_1 & b_2 c_2 \\
 a_1 c_1 & a_1 b_1 c_2 & a_1 b_2 \\
 a_2 c_2 & a_2 b_1 & a_2 b_2 c_1
 \end{array} \quad (210)$$

Greco-Latin squares are used to study four qualitative factors which do not interact. A three-level Greco-Latin square is a one-ninth replicate of a full four-factor design. The corresponding four-level design is a one-sixteenth replicate. In general, an  $m$ -level Greco-Latin square contains  $(1/m)^2$  times the total number of tests in a full four-factor,  $m$ -level factorial design.

A Greco-Latin square may be constructed by selecting two Latin squares having the property that when they are superimposed upon each other, each subscript in one square appears once with every subscript in the other square. Two Latin squares that have this property are said to be orthogonal to each other; for example, squares (208) and (209) are orthogonal and may be superimposed to give

$$\begin{array}{ccc} 0,0 & 1,1 & 2,2 \\ 1,2 & 2,0 & 0,1 \\ 2,1 & 0,2 & 1,0 \end{array} \quad (211)$$

The first subscript in each pair is obtained from the Latin square (209) and the second subscript is from the Latin square (208). Now, let the first subscripts be those of the letter c and the second subscripts be those of the letter d. The array (211) then represents the following nine tests:

$$\begin{array}{ccc} (1) & b_1 c_1 d_1 & b_2 c_2 d_2 \\ a_1 c_1 d_2 & a_1 b_1 c_2 & a_1 b_2 d_1 \\ a_2 c_2 d_1 & a_2 b_1 d_2 & a_2 b_2 c_1 \end{array} \quad (212)$$

This method of constructing the above square gives a design from which the main effects of all four factors can be estimated.

As the number of levels per factor increases, it is possible to find more than two Latin squares which are mutually orthogonal to each other. Such squares form an orthogonal set. To illustrate the usefulness of such squares, consider a metallurgical process which involves four sources of ore,  $X_a$ ; four sources of reagent,  $X_b$ ; four men,  $X_c$ ; operating four similar sets of equipment,  $X_d$ ; and four analysts,  $X_e$ , assaying the products of the process. A full factorial design to test five factors each at four levels requires 1,024 tests. However, three mutually orthogonal, four-level Latin squares may be used to reduce the number of tests to 16. The following three squares

$$\begin{array}{cccc} 0 & 1 & 2 & 3 \\ 1 & 0 & 3 & 2 \\ 2 & 3 & 0 & 1 \\ 3 & 2 & 1 & 0 \end{array} \quad \begin{array}{cccc} 0 & 1 & 2 & 3 \\ 2 & 3 & 0 & 1 \\ 3 & 2 & 1 & 0 \\ 1 & 0 & 3 & 2 \end{array} \quad \begin{array}{cccc} 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 \\ 1 & 0 & 3 & 2 \\ 2 & 3 & 0 & 1 \end{array} \quad (213)$$

may be superimposed to give

$$\begin{array}{cccc} 0,0,0 & 1,1,1 & 2,2,2 & 3,3,3 \\ 1,2,3 & 0,3,2 & 3,0,1 & 2,1,0 \\ 2,3,1 & 3,2,0 & 0,1,3 & 1,0,2 \\ 3,1,2 & 2,0,3 & 1,3,0 & 0,2,1 \end{array} \quad (214)$$



This array is called a hyper Greco-Latin square and represents the following 16 tests:

$$\begin{array}{cccc}
 (1) & b_1 c_1 d_1 e_1 & b_2 c_2 d_2 e_2 & b_3 c_3 d_3 e_3 \\
 a_1 c_1 d_2 e_3 & a_1 b_1 d_3 e_2 & a_1 b_2 c_3 e_1 & a_1 b_3 c_2 d_1 \quad (215) \\
 a_2 c_2 d_3 e_1 & a_2 b_1 c_3 d_2 & a_2 b_2 d_1 e_3 & a_2 b_3 c_1 e_2 \\
 a_3 c_3 d_1 e_2 & a_3 b_1 c_2 e_3 & a_3 b_2 c_1 d_3 & a_3 b_3 d_2 e_1
 \end{array}$$

These tests can be made to estimate the main effects of each of the five factors over the range of four levels for each factor. The data obtained can serve to identify the factor or factors that require more detailed investigation if the process variability is unacceptable.

Several examples of Latin squares containing up to 12 levels per factor and sets of orthogonal Latin squares containing up to 9 levels per factor are given in a book by Fisher and Yates.<sup>13</sup> Examples also are given in books by Davies<sup>14</sup> and by Cochran and Cox.<sup>15</sup>

#### Randomized Designs

The statistical validity of results obtained from any experiment depends upon the tests being made in a random order. If the tests are not made in random order, a trend may appear in the results as a consequence of the order in which the tests are made. Such a trend due to variation in an unobserved factor may contribute to the estimates of some of the important factor effects; for example, wear of equipment can produce a time trend in results obtained.

Since uniform test conditions cannot always be guaranteed, the tests must be made in a random order to minimize the effects of extraneous factors.

There are several ways to randomize the order in which tests are made. One way is simply to randomize all the tests in an experiment; for example, suppose a design requires 16 different tests, and to evaluate experimental error, three full replicates of the design are to be included in the experiment. The numbers from 1 to 48 may be assigned to the tests and then randomized to give the order in which to make the tests.

The order in which to make a series of tests is random if, and only if, it is obtained by a random process such as tossing coins, drawing numbered cards out of a bowl, and the like. Such processes may be time consuming, so tables of random digits have been prepared for use in randomizing the order of a series of tests. When using such a table, a random method is employed

<sup>13</sup>Fisher, R. A., and Yates, F., *Statistical Tables for Biological, Agricultural, and Medical Research*: Hafner Publishing Co., Inc., New York, N.Y., 5th ed., 1957, pp. 80-83.

<sup>14</sup>Davies, O. L., *Design and Analysis of Industrial Experiments*: Hafner Publishing Co., New York, N.Y., 1956, pp. 159-186.

<sup>15</sup>Cochran, W. C., and Cox, G. M., *Experimental Design*: John Wiley & Sons, Inc., New York, N.Y., 1950, pp. 86-121.

for selecting a row and a column in which to find the first digit. A toss of a coin then may be used for deciding whether to read to the right, left, up, or down from this point to obtain a random sequence for the test numbers in the experiment.

The use of a table of random numbers may be illustrated as follows: In most cases, a metallurgical experiment will consist of somewhat less than 100 tests, but often more than 10 tests. Therefore, table 8 was prepared to contain 25 rows and 25 columns of the two-digit numbers from 00 to 99 arranged in a random order.

TABLE 8. - Random numbers

	01 02 03 04 05	06 07 08 09 10	11 12 13 14 15	16 17 18 19 20	21 22 23 24 25
01	86 50 87 87 65	87 13 51 84 13	20 31 76 12 19	85 06 00 70 27	20 68 86 38 51
02	83 27 88 06 02	09 09 21 32 14	37 44 46 18 50	50 54 33 58 45	63 64 65 12 19
03	31 27 62 39 20	21 31 36 27 23	41 44 51 52 25	61 30 66 66 67	68 71 10 71 71
04	75 79 32 81 83	86 54 86 87 88	72 89 86 54 69	89 09 49 51 43	90 06 17 16 49
05	15 75 76 81 87	40 88 54 90 13	68 83 54 73 13	90 91 60 14 46	68 91 17 22 73
06	29 96 95 35 01	91 91 24 94 80	37 29 90 01 59	53 79 24 16 47	05 26 55 59 38
07	80 30 33 03 20	28 47 02 04 15	30 40 49 12 17	70 74 85 48 06	29 60 52 63 26
08	64 69 77 82 83	98 60 99 66 10	17 08 25 30 99	99 85 54 61 72	16 03 14 10 37
09	34 45 85 39 94	43 39 95 11 97	98 18 43 97 97	87 93 67 56 81	21 71 95 08 43
10	90 96 96 96 10	94 96 21 69 24	77 00 09 20 05	57 05 61 93 49	19 45 82 93 95
11	23 38 00 29 74	11 57 30 13 44	47 10 49 36 52	55 57 11 55 64	73 03 56 15 24
12	65 65 28 67 72	22 50 33 38 73	12 74 76 78 38	78 23 73 76 60	70 72 82 28 47
13	48 13 25 56 70	76 05 28 42 68	83 19 15 26 32	12 06 40 44 51	46 70 80 84 03
14	06 64 02 07 15	17 08 27 28 34	41 01 42 44 58	60 42 55 58 67	72 16 47 77 10
15	24 27 35 35 11	35 22 43 00 10	07 31 48 63 50	65 69 62 74 78	56 38 71 52 84
16	66 25 91 52 63	74 52 79 80 97	77 72 78 99 08	79 46 61 34 91	79 29 14 69 56
17	86 52 36 80 30	73 64 88 53 24	80 39 86 14 22	16 36 68 48 90	92 32 18 59 55
18	20 78 75 75 94	65 34 95 09 03	10 39 40 94 25	59 22 19 01 29	95 96 41 62 34
19	02 16 53 75 82	11 92 51 53 82	85 69 56 00 32	35 37 44 48 50	57 33 39 59 43
20	08 25 42 23 04	13 21 34 18 07	33 06 45 60 67	23 42 67 70 75	83 88 31 41 57
21	91 21 92 16 01	04 92 89 26 77	81 92 07 14 18	31 37 62 63 03	42 55 66 66 09
22	12 74 48 48 11	09 46 58 61 46	09 53 76 78 81	82 89 93 10 57	05 33 64 93 62
23	92 89 98 19 97	39 85 62 88 98	99 93 23 94 98	04 08 28 59 63	32 45 79 84 84
24	02 36 04 58 17	21 35 40 40 01	36 41 53 07 15	26 15 05 61 71	37 26 81 00 19
25	41 45 02 77 84	12 30 81 24 18	04 75 58 22 89	07 02 12 47 95	96 97 89 98 49

Now suppose 16 tests are to be made. One convenient way to select the test number is to take any textbook that may be handy and open it to a random page. The even-numbered page will always be on the left-hand side of an open book, so the toss of a coin may decide whether to read the even or odd number. Let the page number so selected be 186. A multiple of 25 (in this case 175) can be subtracted from 186 to obtain 11. This will be the row number. The book may be closed and opened again to obtain the column number, say 18. Now further tossing of the coin may determine that the column should be read down to obtain the sequence

11, 73, 40, 55, 62, 61, 68, 19, 44, 67, etc.

(216)



For convenience, since only 16 tests are involved, subtract a multiple of 20 from each number equal to or greater than 20. This gives the sequence

11, 13, 00, 15, 2, 1, 8, 19, 4, 7, etc. (217)

The numbers 00, 17, 18, and 19 will be ignored. When the bottom of the column is reached, continue at the top of column 19 and read down again. As soon as a number from 1 to 16 has been obtained, it will be ignored when it appears later in the sequence. This procedure is continued until the following sequence is obtained:

11, 13, 15, 2, 1, 8, 4, 7, 5, 12, 10, 6, 14, 16, 3, 9. (218)

The tests are numbered before the sequence is obtained and then made in the order indicated.

When designing a fractional factorial experiment, there are two or more design blocks of tests that can be made. The blocks should be numbered, and one of the blocks then should be selected in a random way. Perhaps more than one system of confounding will yield data that are adequate for a particular experiment. In this example, the number of blocks from which one block may be located is increased. Latin squares are a special case of the latter situation.

With more than three levels per factor in a Latin square, the number of possible squares from which to make a random selection becomes large. For example, there are 576 different four-level Latin square designs and 161,280 five-level Latin square designs. The following procedure can be used to make a random selection from these designs. There are four choices, 0, 1, 2, or 3 for the first value in the first row of the four-level Latin square. Once this choice is made, there are three choices remaining for the second value. Then there are two choices for the third value, and the fourth value is determined by the first three choices. Now, there are three choices for the first value in the second row, and there may be two or three choices for the second value.

This procedure is continued until, finally, all values in the last row are determined by the values previously chosen. Each location in a Latin square must be considered carefully because sometimes the number of choices depends upon the specific values which have been obtained previously. The table of random numbers can be used to select the values for each location. Since there are only four values, the digits may be read singly rather than in pairs. First let 4 = 0, 5 = 1, 6 = 2, 7 = 3, and ignore digits 8 and 9. Then based on a random selection begin in table 8, row 14, column 03 and read to the right. The sequence of digits beginning 0, 2, 0, 7 selects the following values for the first row:

0, 2, 3, 1. (219)

Continuing in this way, the next digits in the sequence, 1, 5, 1, 7, 0 select the values for the second row:



1, 3, 0, 2. (220)

The digits 8, 2, 7, 2, 8, 3, 4 select the first two values, and the third row then is

2, 0, 1, 3. (221)

Finally, the fourth row must be

3, 1, 2, 0. (222)

The digits that are underlined are those which actually determine the corresponding underlined values in each row.

The more information one wishes to obtain from an experiment, the less opportunity there may be to randomize the experiment. If only the main effects of the factors are important, there may be many Latin square designs from which to choose. If a particular system of confounding were required, there may be only two or three design blocks available. When a full factorial design is necessary, there is only one set of tests. In all cases, the tests that are selected or determined by a design should be made in a random order.

#### Randomized Blocks

An ideal experiment would be one in which the factors to be studied could be controlled exactly at the levels specified by the design and all other test conditions could be maintained at constant levels. There would be no need for randomization in research conducted under such conditions. In actual practice, however, this is rarely possible.

A set of tests that can be made under closely controlled conditions is called a block of tests. A man may be able to make eight tests in 1 day. Then those tests constitute a block of eight tests. It may be possible to place four ore samples in a furnace at one time. The four samples treated during a single furnace campaign constitute a block of four tests. If eight samples are to be treated during two different campaigns, the eight tests constitute two blocks of four tests. The tests within any block of tests should be made in a random order.

Randomizing all tests in an experiment is not always sufficient. Consider a design consisting of five tests and an experiment in which each of the design tests is to be made twice. A random order in which to make the 10 tests might be

8, 6, 10, 5, 7, 2, 4, 3, 9, 1. (223)

Test 6 will be the same as test 1, 7 the same as 2, and so on. The order of set (223) may be rewritten as follows:

3, 1, 5, 5, 2; 2, 4, 3, 4, 1. (224)

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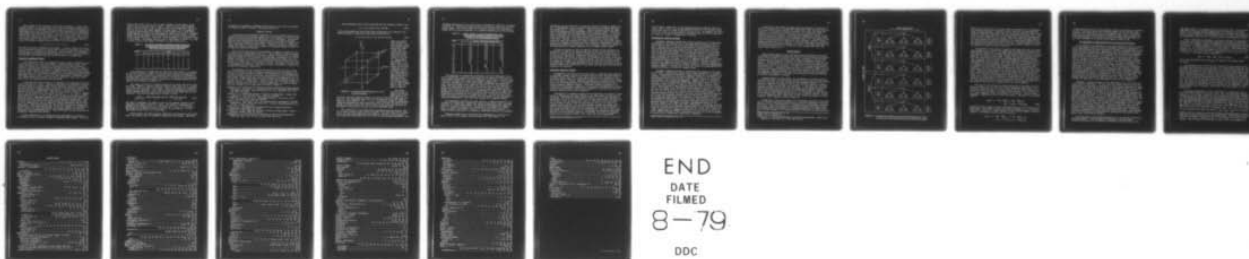
BUREAU OF MINES WASHINGTON D C  
AN INTRODUCTION TO STATISTICAL DESIGN OF EXPERIMENTS IN METALLU--ETC(U)  
1963 S J HUSSEY, P L PLACEK, C H SCHACK  
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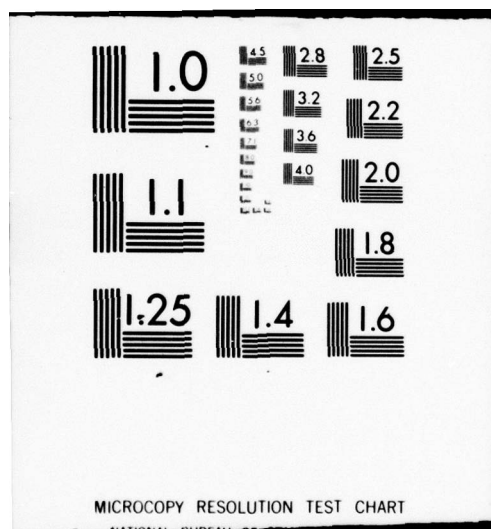
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Now, suppose it were possible to make only five tests at a time. The primary objective of the experiment is to obtain comparisons between the five different tests. The purpose of duplicate tests is to obtain an estimate of experimental error and to determine which of the comparisons are significant when compared with experimental error. The order of set (224) has the disadvantage that test 4 is not included in the first block of five tests. Also, test 5 is not included in the second block. It is preferable to include all five design tests in each block. An example of an order in which the five tests are randomly arranged within each block is the following:

$$2, 1, 5, 4, 3; \quad 5, 2, 3, 1, 4. \quad (225)$$

The above is called a randomized block design. A design, whether full factorial, fractional factorial, or another type, requires a specified set of tests, and this set is a replicate of the design. The requirement of a randomized block design is that each block should contain one or more complete replicates and that the tests within each block should be made in a random order.

#### Incomplete Randomized Blocks

It is desirable to make all comparisons between tests at different factor levels by means of data from tests within a single experiment block. This reduces the chance for variations in extraneous factors from one block to another to influence the estimates of the important factor effects. However, it is not always possible to include a complete replicate of a design in one block of tests. Such a situation is considered in the sections on confounding where the tests of a full factorial design are to be divided among two or more experiment blocks of tests. In each of these experiments a fractional factorial design consists of one-half, one-third, one-fourth, and so on, of the tests in the corresponding full-factorial design.

A situation may arise in which it is desirable to include some other fraction of the tests in a block. Suppose an experiment were designed to investigate five levels of a single factor and for practical reasons it is possible to assure uniform conditions within a block only if each block contains a maximum of four tests. Comparisons between tests at all five levels can be obtained from two blocks of tests. One block can consist of tests  $a_0, a_1, a_2$ , and  $a_3$ , and the second block can consist of tests  $a_0, a_1, a_2$ , and  $a_4$ . Comparisons between tests  $a_0, a_1$ , and  $a_2$  can be made by means of the data from both blocks of tests. Comparisons between test  $a_3$  and the first three tests can be made with the data from the first block, and comparisons between test  $a_4$  and the first three tests can be made with the data from the second block. Test  $a_3$  can be compared with test  $a_4$  indirectly through comparisons with the first three tests. Comparisons between the various tests are made by studying the differences in the responses obtained. In the last example, the responses for tests  $a_3$  and  $a_4$  are each compared with the average response for the first three tests in the appropriate block. These two blocks of tests constitute an incomplete randomized block design.

If all comparisons are to be made with the same degree of precision, it is necessary to use a balanced incomplete randomized block design. In the two

blocks given above, tests  $a_0$  and  $a_1$  appear together in both blocks, so do tests  $a_0$  and  $a_2$  and also tests  $a_1$  and  $a_2$ . Tests  $a_0$  and  $a_3$  appear together only in the first block, tests  $a_0$  and  $a_4$  only in the second block, and so on. Tests  $a_3$  and  $a_4$  do not appear together in either block. For an incomplete randomized block design to be balanced, every possible pair of tests should appear together in a block the same number of times in the design. A balanced design for the experiment to test five levels of a factor in blocks of four tests is given in table 9. Every pair of tests appears in a block three times in this design. For example, tests  $a_0$  and  $a_1$  both appear in blocks 1, 2, and 3; tests  $a_0$  and  $a_2$  both appear in blocks 1, 2, and 4, and so on.

TABLE 9. - A balanced incomplete randomized block design for an experiment consisting of five tests in which four tests are to be made in each block

Block	Test				
	1	2	3	4	5
1	$a_0$	$a_1$	$a_2$	$a_3$	-
2	$a_0$	$a_1$	$a_2$	-	$a_4$
3	$a_0$	$a_1$	-	$a_3$	$a_4$
4	$a_0$	-	$a_2$	$a_3$	$a_4$
5	-	$a_1$	$a_2$	$a_3$	$a_4$

The advantage of a design which is symmetrical with respect to a diagonal of the array as shown in table 9 is that the same statistical procedures can be used to compare the effects of different tests corrected for differences between blocks, and also to compare the effects of different blocks corrected for differences between the tests. However, not all balanced incomplete randomized block designs are symmetrical.

The number of blocks in a balanced design may be larger than in the example given. Suppose a complete replicate requires eight tests and it is possible to make only six tests in each block. There are 28 blocks in a balanced design for this experiment. This number is found by determining how many different combinations of six tests can be obtained from the eight tests in the replicate. The following combinatorial formula is used:

$$\frac{n!}{r!(n-r)!} = \frac{n(n-1)\dots(n-r+1)}{r!} = \frac{n(n-1)\dots(r+1)}{(n-r)!} \quad (226)$$

The letter  $n$  represents the number of tests in the complete replicate, and  $r$  represents the number of tests in a block. The symbol  $n!$  represents the product of all integers from 1 to  $n$  and equals  $n(n-1)(n-2)\dots(3)(2)(1)$ . The second form of equation (226) is used if  $r$  is less than  $(n-r)$ ; the third form is used if  $(n-r)$  is less than  $r$ .

Youden squares and lattice squares, which also are discussed in the literature, are special cases of incomplete randomized block designs. Additional



information on incomplete randomized block designs can be found in the books by Fisher and Yates,<sup>16</sup> Davies,<sup>17</sup> and Cochran and Cox.<sup>18</sup>

### Composite Designs

The degree of the polynomial components of the main effects which can be estimated by using the factorial designs thus far discussed is limited by the number of levels associated with each factor in the experiment. For certain problems this limitation can be overcome by the use of composite designs. These avoid the considerable extra labor involved in the use of a regular factorial experiment with more factor levels. Composite designs are formed by adding extra tests at proper factor levels to a factorial design too small to estimate the effects of interest.

Much work has been done in the development of composite designs for the estimation of all second-degree terms.<sup>19-22</sup> The estimation of the corresponding second order coefficients is the major problem. The procedure for making composite designs for the estimation of second-order coefficients is to first choose a two-level, full-factorial or fractional-factorial design that will provide an estimate of all first order coefficients and such interaction coefficients of second order as are presumed to exist. The design so chosen then is supplemented by additional tests that will make it possible to estimate the second order quadratic coefficients.

The procedure will be illustrated on the basis of the two-level, three-factor full-factorial copper leaching experiment previously discussed in the section on two-level factorial designs. The response for this experiment was recovery of copper, and the factors were percent solids,  $X_a$ , at 25 and 35 percent solids; leaching time,  $X_b$ , at 30 and 40 minutes; and temperature,  $X_c$ , at 25° and 35° C. The design units for these factors were 10 percent solids, 10 minutes, and 10° C., respectively. The base levels were 30 percent solids, 35 minutes' leaching time, and 30° C. leaching temperature. In terms of design units the diagram for this experiment was shown in figure 8.

<sup>16</sup>Fisher, R. A., and Yates, F., Statistical Tables for Biological, Agricultural, and Medical Research: Hafner Publishing Co., Inc., New York, N.Y., 5th ed., 1957, pp. 84-85.

<sup>17</sup>Davies, O. L., Design and Analysis of Industrial Experiments: Hafner Publishing Co., Inc., New York, N.Y., 1956, pp. 199-246.

<sup>18</sup>Cochran, W. C., and Cox, G. M., Experimental Design: John Wiley & Sons, Inc., New York, N.Y., 1950, pp. 259-390.

<sup>19</sup>Box, G. E. P., and Wilson, K. B., On the Experimental Attainment of Optimum Conditions: Jour. Royal Statistical Soc., series B (Methodological), vol. 13, No. 1, 1951, pp. 1-45.

<sup>20</sup>Box, G. E. P., The Exploration and Exploitation of Response Surfaces: Biometrics, March 1954, pp. 16-60.

<sup>21</sup>Davies, O. L., The Design and Analysis of Industrial Experiments: Oliver and Boyd, London, 1954, pp. 532-551.

<sup>22</sup>Andersen, S. L., Statistics in the Strategy of Chemical Experimentation: Chem. Eng. Prog., vol. 55, No. 4, April 1959, pp. 61-67.

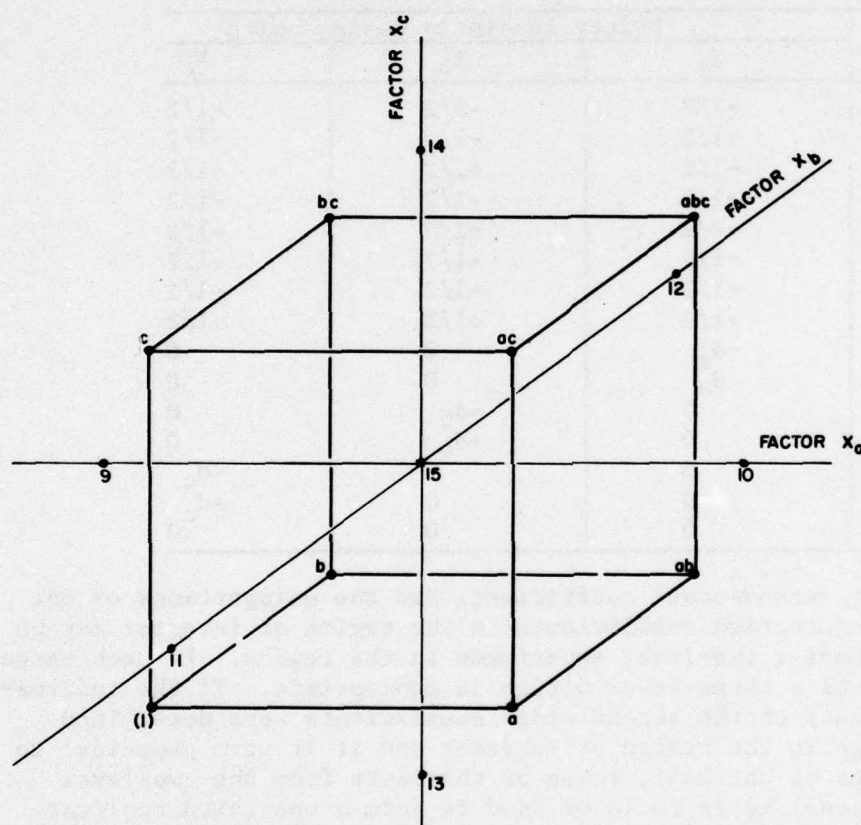


The coefficients that could be obtained from the design of figure 8 are

$$I, A, B, C, AB, AC, BC, \text{ and } ABC. \quad (227)$$

If it were assumed that only second-order coefficients were important, the complete group of coefficients that would be desired are

$$I, A, A^2, B, B^2, C, C^2, AB, AC, \text{ and } BC. \quad (228)$$



There are various ways in which the basic design of figure 8 may be supplemented with additional tests to estimate the quadratic effects and obtain the coefficients  $A^2$ ,  $B^2$ , and  $C^2$ . One possible arrangement is to make a test at the center of the basic design and two tests along each of the coordinate axes of the design spaced at equal intervals in opposing directions from the center. This makes a total of seven additional tests. This arrangement of tests is shown in figure 9.

FIGURE 9. - A Composite Design Based Upon a  $2 \times 2 \times 2$  Factorial Experiment.

The factor levels in terms of design units for the eight tests of the

two-level factorial design in figure 9 are shown in the first eight lines of table 10. The additional seven tests for the composite design are shown in figure 9 by the numbers 9, 10, . . . , 15. If the letter  $d$  with an appropriate subscript represents the axial distances of the tests from the center of the design, the factor levels then will be shown in the latter half of table 10. The values to be given  $d_a$ ,  $d_b$ , and  $d_c$  will be discussed later.

The coefficients in set (228) can be determined from data obtained from the 15 tests listed in table 10 and, therefore, in 12 less tests than a three-level, full-factorial experiment would require. However, if one or more of the interaction coefficients,  $AB$ ,  $AC$ , or  $BC$ , can be considered negligible, the

remaining coefficients of set (228) could be obtained by 9 tests of a one-third replicate of a three-level design instead of the 15 tests required by the composite design. The cases in which the one-third replicate of a three-factor design could be used in preference to a composite design now will be discussed.

TABLE 10. - Factor levels in terms of design units for a three-factor composite design for the estimation of all second-degree effects

Test	Factor levels in design units		
	$X_a$	$X_b$	$X_c$
(1)	-1/2	-1/2	-1/2
a	+1/2	-1/2	-1/2
b	-1/2	+1/2	-1/2
ab	+1/2	+1/2	-1/2
c	-1/2	-1/2	+1/2
ac	+1/2	-1/2	+1/2
bc	-1/2	+1/2	+1/2
abc	+1/2	+1/2	+1/2
9	$-d_a$	0	0
10	$d_a$	0	0
11	0	$-d_b$	0
12	0	$+d_b$	0
13	0	0	$-d_c$
14	0	0	$+d_c$
15	0	0	0

The importance of second-order coefficients and the unimportance of one of the second-order interaction coefficients in the region of interest may be known without having made a two-level experiment in the region. In such cases a one-third replicate of a three-level design is appropriate. If the information about the importance of the second order coefficients were determined from a two-level design in the region of interest and if it were practical to reduce the design units by one-half, three of the tests from the two-level design plus six additional tests could be used to form a one-third replicate design. This also may be done if it is permissible to double the range of the experiment in one direction for one or more of the factors and to reduce the design units by one-half for the remaining factors. In each of these situations involving a three-factor problem, the total number of tests necessary to obtain the information is less than that required by a composite design.

For experiments with more than three factors, a composite design for the estimation of second-order coefficients requires fewer tests than a one-third replicate of a three-level design. For two-factor experiments the number of tests in a composite design for the estimation of all second order coefficients is equal to the number of tests in a three-level full factorial. A useful one-third replicate of a two-factor, three-level design is not possible.

Composite designs may be constructed for experiments in  $k$  factors in a manner similar to the example previously given for three factors. An



appropriate two-level factorial or fractional-factorial design is chosen, and  $2k + 1$  supplementary points are added to the design at the center and along each design axis in a similar fashion. Composite designs provide the advantage of proceeding with the experimental work in natural stages. The factorial or fractional-factorial experiment can be completed first. If the first order coefficients are relatively large compared to the interaction coefficients of second order, the research worker can proceed with the next stage of his work. However, if the interaction coefficients of second order are relatively large (not necessarily larger), compared to the first-order coefficients, the research worker then can add the necessary supplementary points to determine the quadratic coefficients. This advantage is especially helpful in the determination of optimum conditions by the steepest ascent method.

It must be pointed out that in composite designs for the estimation of coefficients as high as the second order some of the coefficients that it is desired to estimate will be biased by higher order aliases if some of these aliases are not negligible. Third-order coefficients are the most likely to be troublesome, and if some of them are not negligible, the extent of the bias will vary with the type of the composite design. The choice between a composite design and a higher level factorial must be based upon an evaluation of the importance of conserving experimental effort and the consequences of being wrong if higher order coefficients are actually more important than previously estimated or stipulated.

#### Orthogonal Composite Designs

Orthogonality previously has been set forth as a desirable characteristic of experiment designs, because such designs provide effect estimates which are uncorrelated with each other in that the variations of the estimates of the individual effects within the experimental region are not artificially related due to the manner of design. Composite designs may be arranged so that orthogonality of the estimated effects is thereby insured and such designs are called orthogonal composite designs. Orthogonal composite designs for the estimation of second-order coefficients also provide a minimum amount of possible bias from third-order coefficients as compared to the effects of bias in composite designs which are not orthogonal.

Orthogonality in composite designs for the estimation of quadratic coefficients is obtained by the proper spacing of the extra points on each axis of the design. The composite design shown in figure 9 can be made orthogonal by making tests 9, 10, 11, 12, 13, and 14 at the same distance from the center of the design in terms of design units; that is, the factor levels for these tests as shown in table 10 must be such that  $d_a = d_b = d_c = d$ , when  $d$  is a properly chosen constant. For two-level designs in which the design unit is one-half the distance between the two levels of a factor, Box and Wilson<sup>23</sup> have listed the proper values of  $d$  for orthogonality. For two-, three-, and four-factor full factorials and for a five-factor, half-replicate fractional factorial with the defining contrasts I and ABCDE, the proper corresponding values of  $d$  are listed as 1.000, 1.215, 1.414, and 1.547, respectively.

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<sup>23</sup>Work cited in footnote 19, p. 37.



In this paper a design unit is the distance between two adjacent levels of a factor, and for such a case the corresponding values of  $d$  are one-half those given above; that is, 0.500, 0.608, 0.707, and 0.774. For example, the values of  $d_a$ ,  $d_b$ , and  $d_c$  in the three-factor composite design of table 10 should be  $d_a = d_b = d_c = 0.608$  if orthogonality is desired.

#### Nonorthogonal Composite Designs

Orthogonal composite designs that provide estimates of all second-order coefficients do not estimate all of the second-order coefficients with the same precision; that is, the errors associated with the estimates are not equal. Specifically the errors in the quadratic coefficients and those in the second-order interaction coefficients are respectively equal, but the error in the quadratic coefficients is larger than the error in the second order interaction coefficients. In some research problems it is desirable that all second-order coefficients be estimated as nearly as possible with equal precision, and this only can be accomplished at the expense of not having orthogonality in design. It also is sometimes desirable to use composite designs in which the extra tests are not added to the basic factorial design in the symmetrical fashion shown in figure 9. Composite designs that meet the requirements of these two general situations are called nonorthogonal composite designs. Problems such as these can arise in the determination of optimum conditions by the path of steepest ascent.

Orthogonal composite designs are symmetrical with respect to the center of the design. Nonorthogonal designs may be either symmetrical or nonsymmetrical. In nonorthogonal symmetrical composite designs for the estimation of quadratic coefficients, one or more of the pairs of tests on the factor axes are placed at factor levels that are farther from the center of the design than necessary for obtaining orthogonality. However, when it is desired to estimate all of the second-order coefficients with equal errors, it also is necessary to make all pairs of tests on the factor axes at specific factor levels that are placed at equal distances from the center in terms of design units. With regard to the three-factor design shown in table 10, it is necessary that the factor levels of tests 9 to 14, inclusive, should be such that  $d_a = d_b = d_c = d$ , where  $d$  is a certain value for three-factor designs. For composite designs in which the basic two-level factorial design has units that are one-half the distances between levels of the factors, Box and Wilson<sup>24</sup> have listed the proper values of  $d$  necessary to obtain equality of errors for all second-order coefficients. For two-, three-, and four-factor full factorials and for a five-factor half-replicate fractional factorial with the defining contrasts I and ABCDE, the proper corresponding values of  $d$  are listed as 2.090, 2.432, 2.799, and 2.872, respectively. For designs in which the units are equal to the distances between levels of the basic factorial the values of  $d$  are one-half those just given; that is, 1.045, 1.216, 1.400, and 1.436, respectively; for example, the values of  $d_a$ ,  $d_b$ , and  $d_c$  in the three-factor composite design of table 10 should be  $d_a = d_b = d_c = 1.216$  if equality of errors for all second order coefficients is desired.

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<sup>24</sup>Work cited in footnote 19, p. 37.

Inspection of the values of  $d$  given by Box and Wilson<sup>25</sup> for equality of errors in estimates of all second-order coefficients shows that the values of  $d$  increase as the number of factors increases. The values of  $d$  range from 2.090 for a two factor full factorial to 2.872 for a five-factor half-replicate of a full factorial. The absence of orthogonality results in correlation between the estimates of the quadratic coefficients, and the amount of such correlation increases with increasing values of  $d$ . The amount of possible bias from third-order coefficients also increases. Davies<sup>26</sup> cautions against using values of  $d$  as large as 3 because the magnitude of possible bias from third-order coefficients becomes too serious. For design units equal to the distance between levels of the factors, the limiting value which may cause trouble would be 1.5.

### Nested Designs

Nested designs generally are used when successive sampling is necessary to determine by subsequent testing the variation in some associated characteristic of the material or condition under study. Estimates of the variation introduced by the successive stages of the sampling procedure usually are desired. Nested designs may be either balanced or unbalanced. When the same number of replications occur within each replication of the preceding stage, the design is said to be balanced. An example of a balanced nested design is shown in figure 7. Balanced designs may require a prohibitive number of tests to obtain an accurate estimate of the desired variation in the first stage of the sampling. Unbalanced designs are often more efficient for this purpose, and mathematical methods are available for assessing the relative efficiency of possible arrangements in design.<sup>27</sup>

Sampling schemes, however simple, are experiments or fractions thereof with nested designs. All statistical methods are based upon the proper manipulation of data that have been obtained by some sampling procedure. It is, therefore, important in design to take due note of those aspects of sampling that have a direct bearing upon any experiment. In some cases the necessary sampling procedures do not enter into the design of the experiment but are a mode of operation necessary to perform the experiment properly. However, recognition of sampling problems may result in a design that includes factors due to sampling even though such factors are not of primary concern. In such a case the design may have a model that is both crossed and nested in classification. Such a design is shown in figure 10.

Designs such as the one in figure 10 are sometimes used when it is necessary to introduce sampling procedures into a factorial experiment in which the influence of two or more factors of a treatment must be introduced in successive stages. Figure 10 illustrates a hypothetical design that might be used in the preliminary investigation of alternative methods for the leach treatment of large tonnages of ore having considerable variation in characteristics.

<sup>25</sup>Work cited in footnote 19, p. 37.

<sup>26</sup>Work cited in footnote 21.

<sup>27</sup>Davies, O. L., Statistical Methods in Research and Production: Hafner Publishing Co., New York, N.Y., 1957, pp. 115-117.



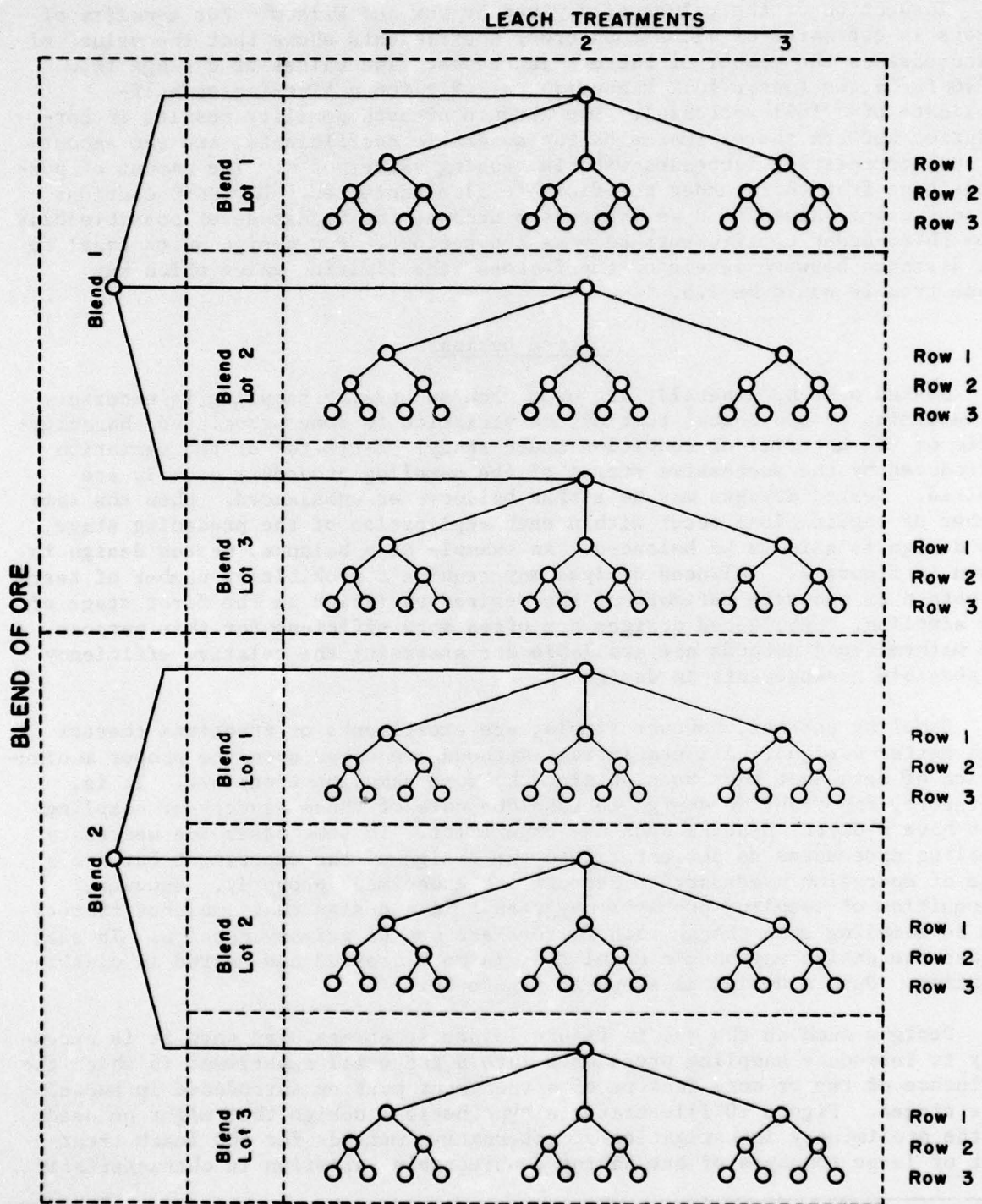


FIGURE 10. - A Design Involving Both Crossed and Nested Classifications. Row 1, leach lots; row 2, leach residue samples; row 3, analytical test samples.



There are two blends of ore, and each blend was considered to be nonhomogeneous and hence was randomly sampled for three blend lots to investigate the effect of nonhomogeneity. Each blend lot was randomly sampled to obtain three leach lots which are indicated by the three small circles in each row 1. The leach lots were subjected to one of the three leach treatments corresponding to the column in which they are located. After the leach treatments each of the leach residues was randomly sampled for two leach residue samples, which are indicated by the small circles in each row 2. Duplicate samples for chemical analysis were removed from each of the leach residue samples, and these are shown by the small circles in each row 3.

An inspection of the design in figure 10 will make clear that the design relationships are as follows: The analytical test samples are nested in the leach residue samples; the leach residue samples are nested in the leach residues from the leach lots; the leach lots are nested in the blend lots; and the blend lots are nested in the blends. However, the variation between leach lots from a particular blend lot is confounded with the variation between leach treatments in such a manner that their combined variation is the variation between the leach residues. Since each blend lot is considered to be well mixed, the variation between the leach lots from a particular blend lot is considered to be insignificant compared to the variation between leach treatments. Therefore, the variation between the leach residues from a particular blend lot is considered to be due solely to the effect of leach treatments. The leach residue samples are nested within leach residues specified by a particular leach treatment, a particular blend lot, and a particular blend. As a result of these conditions, the nesting of the leach lots in the blend lots is ignored for the purposes of design and analysis, and the leach residues are not considered to be nested in the blend lots. The blend lots are cross classified with the leach treatments for each separate blend of ore. The blends of ore are cross classified with the leach treatments.

The model for this crossed and nested design may be developed after the factors, levels, and replicates are suitably designated symbolically. Let the factor symbols  $X_a$ ,  $X_b$ ,  $X_c$ , and  $X_d$ , respectively, represent blends of ore, blend lots, leach treatments, and leach residue samples. Let the letters  $i$ ,  $j$ ,  $k$ , and  $m$  represent levels corresponding to the factors. Let the letter  $n$  represent a numbered replicate of the test samples. The model for the design then is

$$y_{ijkmn} = \mu + *A_i + *B_j(i) + *C_k + *D_m(ijk) + *I_{ik} + *I_{jk(i)} + *e_{n(ijkm)}. \quad (229)$$

A specific chemical analysis may be subdivided into parts on the basis of the model (229). For example, consider the chemical analysis,  $y_{12122}$ , obtained for blend 1, blend lot 2, leach treatment 1, leach residue sample 2, and test sample 2. The chemical analysis may be written as

$$y_{12122} = \mu + *A_1 + *B_2(1 \dots) + *C_1 + *D_2(121 \dots) + *I_{1.1.} + *I_{.21.(1 \dots)} + *e_{2(1212)}.$$

In this equation the dots in the subscripts of some of the terms are essential in order to precisely locate the individual numbers in the subscript with respect to the succession of letters and numbers,  $ijklm = 1212$ . It should be noted that the cross classification of blend lots with leach treatments for each separate blend of ore causes the interaction effect between blend lots and leach treatments to be nested within separate blends of ore.

#### The Importance of Experimental Error in Design Considerations

In the design of an experiment all available information about the nature of the experimental errors that may be encountered should be considered to assure obtaining data that when analyzed will produce the maximum useful information for the work performed. Experimental error may originate from several sources and with suitable experimental designs may be divided into components corresponding to their origin. To illustrate, the error in an observation might be due to the method of measurement, such as analytical error, and also to the manner of conducting the experiment in the laboratory. In most cases an estimate of the total error from all such sources is obtained from all tests as the estimated experimental error. A critical inspection of the sources of error is not made unless this becomes essential in attempts to reduce the size of the experimental error. In this illustration a presumed high degree of precision in a research laboratory might lead one to suspect that errors in chemical analysis were responsible for a considerable portion of the experimental error. A resolution of this suspicion would be essential in deciding how a reduction in experimental error could be accomplished. In this case each test would be performed two or more times, and two or more chemical analyses then would be made for each test. This procedure makes possible the separation of the experimental error into two components.

Sometimes a suitable estimate of the experimental error exists from previous records or experience. In such cases this estimate may be used in the evaluation of the accuracy of observations or the relative importance of experimental effects. When previous estimates of experimental error are not suitable, the experiment may be designed so as to obtain an estimate from the experiment. Sometimes one or more of the possible highest order interactions are known to be nonexistent or statistically unimportant as determined by the analysis of previous data. If so, the experiment can be designed so that such possible highest order interactions are not confounded with other effects, and these interactions then will provide an estimate of the experimental error when the data are analyzed. When all possible interactions are known to exist, it may be necessary to obtain an estimate of the experimental error by making two or more replications of each test. Multiple replication also is often necessary when the number of possible interactions that are nonexistent are too few to give an accurate estimate of the experimental error. Whenever an estimate of experimental error is obtained from an experiment, some consideration should be given to the possibility of combining it with previous estimates to get a more precise estimate.

The basic purpose of multiple replication is to increase the precision of estimating effects. If this purpose is fulfilled in any experiment, increased replication for the purpose of obtaining a better estimate of the



experimental error is an unnecessary waste of time and labor. The precision with which effects are estimated depends upon the relative sizes of the effects to be estimated and the experimental error involved. The smaller an effect is when compared to the experimental error, the better the estimate of the experimental error must be to insure precision in estimating the effect.

When an experiment is designed by statistical methods, the experimental errors that are associated with each observation are assumed to be random variables. For example, consider the manganese flotation experiment in which the response is manganese recovery and the factor  $X_a$  is conditioning time with levels  $k = 1, 2, 3$  corresponding to 3, 4, and 5 minutes' conditioning time, respectively. The factor  $X_b$  is temperature with levels  $m = 1, 2, 3, 4$  corresponding to 30°, 40°, 50°, and 60° C., respectively, and the replicates are  $r = 1$ , and 2. The model for this experiment is

$$y_{kmr} = \mu + *A_k + *B_m + *I_{km} + *e_{r(km)}. \quad (230)$$

All of the experimental errors  $*e_{r(km)}$  are assumed to be random in their occurrence.

The assumption also is made that the random error terms associated with the manganese recoveries of each replicate are uncorrelated and that the random error terms associated with each level of a factor are uncorrelated. This means that variations in test conditions that are beyond control have caused the individual errors in such a manner that they are unrelated in their occurrence. Correlation between errors may result from the effect of some additional factor, which has been ignored but which has influenced the replicates of a test or the results of tests from level to level of a factor in the same way. The control or elimination of such factors is not always possible. However, the effect of such factors upon the validity of the subsequent analysis may be minimized by randomization in the execution of the experiment. Randomization ensures that, in general, such factors contribute equally to each observation.

In designing experiments it also is important to consider what may be known about the variance of the error terms. Since the statistical concept of variance has not yet been introduced, it now will be described with reference to observations and their errors. An understanding of this concept is essential for developing designs that will yield experimental data suitable for the most profitable analysis. If several replicates of a single test are made for the experiment with the model (230), the observations,  $y_{kmr}$ , will have a mean,  $\bar{y}_{km}$ , which is an estimate of the true mean,  $\mu_{km}$ . Each observation will have a deviation from the true mean which is  $*e_{r(km)} = y_{kmr} - \mu_{km}$ . If a large number of such replicates were made, the quantity  $\sum_{r=1}^n (y_{kmr} - \mu_{km})^2 / n$  as  $n$  becomes

infinite would be a measure of the true variation associated with the observations and is called the variance of the observations. This variance is represented by the symbol  $\sigma^2(y_{kmr})$  and also is the variance of the error terms,  $*e_{r(km)}$ . When designing the experiment for model (230), the assumption is



made, unless there is contrary evidence, that the variance of the error terms is equal for all levels of conditioning time and for all levels of temperature. When the condition of equality in variance exists, the error variance is said to be homogeneous.

In the subsequent analysis of the data it is desirable that the variances of the mean values of the observations for the replicates of each test should be equal. In the case of the model (230) the variance of the mean value,  $\bar{y}_{km}$ , for  $n$  replicates of the same test is represented by  $\sigma^2(\bar{y}_{km})$ , and its relationship to  $\sigma^2(y_{kmr})$  is

$$\sigma^2(\bar{y}_{km}) = \sigma^2(y_{kmr})/n. \quad (231)$$

When homogeneity of variance in the observations exists, homogeneity of variance in the observation means also will exist for the usual case of an orthogonal design in which all tests have the same number of replicates. A condition of nonhomogeneity in expected error variance must, therefore, be considered when following the principles of experimental design previously set forth. An illustration of an experiment in which the expected error variance is nonhomogeneous and the design precautions which are useful for obtaining homogeneous observation means now will be presented.

Consider the research problem in the flotation of manganese at the levels of conditioning time and temperature previously given for model (230). Suppose that the results of previous research showed that the estimated variance of the experimental error for manganese recovery with 4 and 5 minutes' conditioning time was approximately, and respectively, two and three times the variance with 3 minutes' conditioning time; that is,

$$\sigma^2(y_{3mr}) = 3\sigma^2(y_{1mr}), \quad (232)$$

$$\sigma^2(y_{2mr}) = 2\sigma^2(y_{1mr}). \quad (233)$$

The variances of the mean values of the observations at the  $m$ 'th level of temperature for levels  $K = 1, 2, 3$  of conditioning time according to equation (231) are, respectively,

$$\sigma^2(\bar{y}_{1m}) = \sigma^2(y_{1mr})/n_1, \quad (234)$$

$$\sigma^2(\bar{y}_{2m}) = \sigma^2(y_{2mr})/n_2, \quad (235)$$

$$\sigma^2(\bar{y}_{3m}) = \sigma^2(y_{3mr})/n_3, \quad (236)$$

wherein  $n_1$ ,  $n_2$ , and  $n_3$  are the number of replicates at levels  $i = 1, 2, 3$ , respectively. For subsequent analysis the desired result is that

$$\sigma^2(\bar{y}_{1m}) = \sigma^2(\bar{y}_{2m}) = \sigma^2(\bar{y}_{3m}). \quad (237)$$

From the relationships of equations (232) to (237) it may be shown that (237) will be so only if  $n_3/n_1 = 3$  and  $n_3/n_2 = 3/2$ . Under the stipulated condition that equations (232) and (233) are approximately true, the use of these ratios

in replication at successive levels of conditioning time will result in a close approximation of the relationships in (237).

In general, if there were prior evidence of nonhomogeneity in variance from level to level of a factor, it should be possible to arrange an experiment so that homogeneity of variance for the mean values of the test replicates is obtained. Furthermore, an experiment with proportionate replication from level to level of a factor is orthogonal, and the effects may be estimated without correlation of the effect estimates.

There are some cases of nonhomogeneity in variance for which precautions are not necessary because it is possible and more practical to use suitable procedures in the analysis of the data to correct the situation. The conditions for which this is so are those where there is an observed relationship between the observation means and the error variance of the observations. The nature of this relationship sometimes may be obtained from prior data by plotting the estimated error variance of the observations against the observation means. Homogeneity of variance in the means of transformed observations then may be obtained in subsequent analysis by substituting a function of the response for the response itself. In general, when there is a known mathematical transformation of the response that will stabilize the variance of the transformation means, the design of the experiment may be conducted by the principles previously set forth without any attempt to incorporate into the design features to correct nonhomogeneity of variance in the subsequent experimental results. Information concerning the types of transformations discussed here may be found in the literature.<sup>28-31</sup>

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<sup>28</sup>Bartlett, M. S., The Use of Transformations: *Biometrics*, vol. 3, No. 1, March 1947, pp. 39-52.

<sup>29</sup>Kendall, M. G., *The Advanced Theory of Statistics*: Hafner Publishing Co., New York, N.Y., vol. 2, 3d ed., 1951, pp. 206-209.

<sup>30</sup>Davies, O. L., *Design and Analysis of Industrial Experiments*: Oliver and Boyd, London, 1954, pp. 44-45.

<sup>31</sup>Bennett, C. A., and Franklin, N. L., *Statistical Analysis in Chemistry and the Chemical Industry*: John Wiley & Sons, Inc., New York, N.Y., 1954, pp. 355-357.



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